

Institute of Science and Technology

Master of Science in Chemistry

M.Sc. Chemistry

Curriculum

1999



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TEXT BOOK

Master of Science in Chemistry
M.Sc. Chemistry

Effective from 1999

Office of the Dean
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Tribhuvan University
Kathmandu, Nepal

TEXT BOOK



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Introduction:

Three-year Bachelor level education (previously two years') has recently 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 undertaking 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 for Admission:

The candidates 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 Central Department of Chemistry. 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 the percentage of marks in their B. Sc. Examination and the 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.

Course Structure:

There are be two academic sessions (part I and part II) each of one year's duration. The total marks allotted are 1000. Theoretical papers carry 100 marks each with the exception of elective papers and research methodology. Each theoretical paper is taught for four hours a week.

Eight hours per week are allotted for the laboratory course carrying 50 marks and twelve hours per week are allotted for dissertation and the laboratory course carrying 75 marks.

The structure of the course for the Master's degree will be as follows:

First Year:

Subjects	Course Number	Full Marks	Pass Marks
Inorganic Chemistry	Chem 511	100	40
Physical Chemistry	Chem 512	100	40
Organic Chemistry	Chem 513	100	40
Research Methodology	Chem 514	50	20
Inorganic Chemistry Practical	Chem 515	50	20
Physical Chemistry Practical	Chem 516	50	20
Organic Chemistry Practical	Chem 517	50	20

Submission of a Term Paper in Research Methodology course is a prerequisite to appear in the first year final examination.

Second Year:

On completion of M.Sc. (Chemistry) Part I, the students have the option of specializing either in Organic, or Physical or Inorganic Chemistry in M.Sc. (Chemistry) Part II program.

There are three papers each of 100 marks in every specialized subject, 75 marks for an elective subject and 50 marks for compulsory practical and 75 marks for practical or Dissertation. Participation in **Seminar is a compulsory non-credit course. Regular attendance and presentation of the assigned topic at the seminar is a prerequisite to appear in the final examination.** The details of the Course Numbers for each subject and the corresponding marks are given below:

Inorganic Chemistry

Subjects	Course Number	Full Marks	Pass Marks
Reaction mechanism, bonding and structure	Chem 611	100	40
Selected topics in inorganic chemistry	Chem 612	100	40
Organometallics and bioinorganic chemistry	Chem 613	100	40
Inorganic Chemistry Practical I	Chem 614	50	20
Inorganic Chemistry Practical II	Chem 615	75	30
Dissertation	Chem 616	75	30

Of the laboratory courses, Chem 614 is compulsory. There is option between Chem 615 and Chem 616 (Dissertation).

Physical Chemistry

Subjects	Course Number	Full Marks	Pass Marks
Quantum and statistical mechanics	Chem 621	100	40
Electrochemistry and solid state chemistry	Chem 622	100	40
Spectroscopy, surface chemistry and group theory	Chem 623	100	40
Physical Chemistry Practical I	Chem 624	50	20
Physical Chemistry Practical II	Chem 625	75	30
Dissertation	Chem 626	75	30

Of the laboratory courses, Chem 624 is compulsory. There is option between Chem 625 and Chem 626 (Dissertation).

Organic Chemistry

Subjects	Course Number	Full Marks	Pass Marks
Organic Synthesis	Chem 631	100	40
Organic reaction mechanism	Chem 632	100	40
Stereochemistry and Spectroscopy	Chem 633	100	40
Organic Chemistry Practical I	Chem 634	50	20
Organic Chemistry Practical II	Chem 635	75	30
Dissertation	Chem 636	75	30

Of the laboratory courses, Chem 634 is compulsory. There is option between Chem 635 and Chem 636 (Dissertation).

Elective Subjects: One of the following subjects must be taken:

Subjects	Course Number	Full Marks	Pass Marks
Spectroscopy	Chem 641	75	30
Nuclear Chemistry	Chem 642	75	30
Natural Product Chemistry	Chem 643	75	30
Food Chemistry	Chem 644	75	30

Visits to industries or educational institutes will be arranged, as deemed necessary, as a part of extra curricular activities.

Course Duration:

The entire course is spread over two academic years. There is a separate annual examination after the end of each academic year.

Hours of instruction:

- a) Working days : 150 days in an academic year.
- b) Class hour :
- i) Theory: One theory paper of 100 marks will have 4 hours lecture per week.
 - ii) Practical: One practical paper of 50 marks will have 8 hours of practical per week and that of 75 marks will have 12 hours of practical per week.

c) Attendance : 70 percent attendance in the class is required.

Examination:

All the students are to appear in four hours' examination for theoretical courses carrying 100 marks as well as 75 marks and it six hours practical examination for 50 marks. Twelve hours' practical examination is for students who opt for a laboratory course in lieu of dissertation in each of the branches. The practical examination for regular laboratory course will be held immediately after the completion of the courses. Schedules for the practical examinations will be announced by the central Department of Chemistry with the approval of the Dean's Office.

Evaluation :

Institute of Science and Technology, Tribhuvan University will conduct annual examinations. The students will have to pass each course at each level separately. The minimum pass marks is 40 percent both for theory and practical.

A student having passed his / her two years of study will be graded as below on the basis of the average marks received in the two years:

75 percent and above Distinction
60 percent and above First Division
50 percent and above Second Division
40 percent and above Third Division

Inorganic Chemistry

Course Title: Inorganic Chemistry
Course No.: Chem 511
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : I

Course Objective : To provide a broad knowledge of the advanced inorganic chemistry and the principles of qualitative and quantitative analysis.

Course Contents:

- Atomic Structure:** Matter waves, the uncertainty principle, the wave nature of electron, interpretation of the wave function, normalized and orthogonal wave functions, the wave equation, the principle of superposition, the particle in a one-dimensional box, the particle in a three-dimensional box, degeneracy, the hydrogen atom, transformation of co-ordinates, 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 **18 hrs.**
- Covalent bond:** The variation method, ground state energy of the hydrogen atom, the Secular equations **4 hrs.**
- Molecular orbital theory:** Molecular orbitals, L.C.A.O. approximation, significance of the resonance, integral, hydrogen molecule ion H_2^+ hydrogen molecule, homonuclear, diatomics (correlation diagrams), heteronuclear diatomics, polarity of orbitals, types of molecular orbitals, iso electronic principle **10 hrs.**
- Valence bond theory:** Valence bond method, the hydrogen molecule H_2 , other homonuclear diatomics, heteronuclear diatomics, quantum mechanical structure and the meaning of resonance, dipole moments, ionic-covalent resonance energy **8 hrs.**
- Hybridization:** sp^3 hybridization, d^2sp^3 hybridization, trigonal and digonal hybrids, non-equivalent hybrids, strength of a hybrid bond, calculation of valence angles **8 hrs.**
- Radio-activity and nuclear reaction :** Characteristics of nuclear reactions and their similarity with chemical reactions, types of nuclear reactors, fission-probability, process yield and applications and fall out, nuclear reactors, classification of reactors, units and measurement of radioactivity and radiation, activation analysis, ^{14}C dating, tracer technique, radiochemical analysis. **10 hrs.**
- Co-ordination compounds:** Crystal field theory: elements of symmetry, symmetry operations, point groups, square planar, octahedral, tetrahedral complexes, relative order of orbital energies for these geometries, crystal field stabilization energy, spectrochemical series, nephelauxetic series, structural effects of CFSE in t_d , O_h , Jahn Teller effect in octahedral complexes, dynamic Jahn Teller behavior, thermodynamic effect of CFSE, enthalpies of hydration of M^{+2} ions, lattice energies of MCl_2 compounds, explanation of magnetic

- properties, color of transition metal complexes, characterization of coordination compounds. **17 hrs.**
- Non-aqueous solvents:** Solvents properties, donor and acceptor properties (solvent polarity), protic and aprotic solvents, types of reaction, reactions in H_2SO_4 , HF, N_2O_4 . **10hrs.**
- ✓ **Electronegativity** : Different scales of electronegativities, variation of electronegativity, choice of electronegativity system, group electronegativity, electronegativity equalization **4 hrs.**
- ✓ **Electron affinity and Ionization energy:** Anomalous electron affinity and ionization energy **3 hrs.**
- Bond energy:** Intrinsic bond energy, mean bond energy. ✓ **3 hrs.**
- ✓ **Hydrogen bonding:** Theory for hydrogen bonding, evidence for hydrogen bonding, consequences of hydrogen bonding, hydrogen bonding involving charged species. **4 hrs.**
- ✓ **Metallic bonding:** Bonding in metals, metal, insulators and conductors, superconductivity. **3 hrs.**
- ✓ **Buckminster Fullerene:** Preparation, endohedral complexes, higher fullerenes. **3 hrs.**
- ✓ **Qualitative and quantitative analysis:** Uses of common organic reagents (dmg, oxine, cupferron, EDTA), redox titration, use of potassium bromate, feric salts, adsorption, redox, and metal ion indicators; Instrumentation, working principles and applications of atomic absorption spectrophotometry, atomic absorption, emission and fluorescence spectrophotometry, flame photometry, emission spectroscopy and thermogravimetric analysis (T.G.A., D.T.A.) **15 hrs.**

Reference Books:

1. F.A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry; 5th ed.*, John Wiley and Sons Ins. (1988) ✓
2. F.A. Cotton, G. Wilkinson and Paul L. Gaus, *Basic Inorganic Chemistry; 3rd ed.*, John Wiley and Sons Incorporation (1995)
3. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic chemistry; 4th ed.* Harper Collins College Publishers (1993) ✓
4. Bodie Douglas, Darl McDaniel and John Alexander, *Concepts and Models of Inorganic Chemistry; 3rd ed.*, John Wiley and Sons Incorporation (1994) ✓
5. M.C. Day and J. Selbin, *Theoretical Inorganic Chemistry*; East-West Press Pvt. Ltd. (1985)
6. C.A. Coulson, *Valence*; E.L.B.S. (1975)
7. E. Cartmell and G.W.A. Fowles, *Valency and Molecular Structure; 4th Ed.* Butterworth (1977)
8. L.F. Audrieth and J. Kleinberg, *Non-aqueous solvents*; Wiley, New York, Latest ed.
9. Ed J.J. Lagowski, *The Chemistry of Non-aqueous Solvents*; Academic Press, New York
10. R. McWeeny, *Coulson's Valence*; Oxford Press (1979)
11. L. Pauling, *The Nature of the Chemical Bond, latest ed.*; Cornell University Press

12. P.J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry; Wiley (Interscience), New York
13. A.F. Wells, Structural Inorganic Chemistry; 4th ed. Clarendon, Oxford (1975)
14. R.A. Day and A.L. Underwood, Quantitative Analysis; 6th ed Prentice-Hall of India (1993)
15. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Textbook of Quantitative Chemical Analysis; E.L.B.S. (1994) 545/V862
16. H.H. Willard, L.L. Merritt, J.R. Dean and F.A. Settle, Instrumental Methods of Analysis; 6th ed Van Nostrand (1981)
17. D.A. Skoog, Principles of Instrumental Analysis; 3rd ed. Saunders College Publishing (1985)
18. H.J. Arnikar, Essentials of Nuclear Chemistry 4th ed; Wiley Eastern Limited. (1995)

Physical Chemistry

Course Title: Physical Chemistry
Course No.: Chem 512
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : I

Course Objective : To provide advanced knowledge on important topics of physical chemistry together with electroanalytical techniques and spectroscopy.

Course Contents:

Mathematics for Chemistry (non-credit course): Derivative and its physical significance, basic rules for differentiation (without derivation), maxima minima and their application in chemistry, exact and inexact differentials with specific emphasis on thermodynamic properties, partial differentiation, basic rules of integration (without derivation), definite and indefinite integration, geometric meaning of integration – application in chemistry, differential equation, concept of boundary values, algebra and elementary concept of function, plotting functions (straight-line, parabola, and logarithm) arithmetic and geometric series, determinants, matrices. **12 hrs.**

Chemical Kinetics:

Fast reactions: Methods used in the study of fast reactions: flow methods, relaxation methods, flash photolysis, NMR, polarographic and other related techniques. **Polymerization reactions:** Addition and condensation polymerization, molecular mechanism, free radical mechanism, cationic, anionic and emulsion polymerization, degree of polymerization, statistics of polymerization. **Oscillating reactions:** Lotka-Volterra mechanism of chemical oscillation, Brusselator and Oregonator, bistability, chemical chaos. **Enzymes catalyzed reaction:** Catalysis by enzymes, Michaelis-Menten mechanism of enzyme action, influence of pH and temperature in enzyme action. **Molecular reaction dynamics:** Diffusion controlled reactions in solution, kinetic salt effect, electron transfer reactions, reaction in molecular beam, potential energy surfaces, attractive and repulsive surfaces, classical trajectories. Photochemistry of air and air pollution. **22 hrs**

Electrochemistry: Ionics:

Ion solvent interaction: Non-structural and structural treatment of ion solvent interaction, solvent number, dielectric constant of water and ionic solution.

Ion-ion interaction: Debye Huckel theory of ion-ion interaction, activity coefficient and ion-ion interaction, the limitation of Debye-Huckel theory of activity coefficient. **The electric double layer:** Elementary idea of Helmholtz, Gouy-Chappman and Stern models.

Electroanalytical chemistry: Polarography (DC), a brief account of: AC, pulse, differential pulse Polarography, instrumentation and applications. Amperometry and amperometric titration, advantage and limitation of amperometric titration, coulometry and coulometric titration, Karl Fisher titration, electrogravimetry, ion selective electrodes: glass and solid state membrane electrodes, analysis with ion selective electrodes. **26 hrs**

Thermodynamics: Pressure, temperature and concentration dependence of equilibrium, LeChatelier's principle. chemical potential of pure substance, chemical potential of substances in mixture, fugacity, relation between fugacity and pressure, determination of fugacity, partial molar quantities, thermodynamics of mixing, colligative properties. 20 hrs

Molecular Statistics & Statistical Thermodynamics: Brief resum'e of the concept of distribution of energy, limitation of classical thermodynamics, statistical treatment of entropy, Boltzmann distribution law, application of Boltzmann distribution law, partition function and its significance, translational, rotational, vibrational and electronic partition functions, thermodynamic properties from partition functions. 18 hrs

Solid State Chemistry:

Lattice energy of ionic solids, classical free electron theory of metals, electrical conductivity Ohm's law, Widemann-Franz ratio, heat capacity of conduction electrons, drawbacks of classical free electron theory, defects in solid structure: point defects, line defects and plane defects. 12 hrs.

Spectroscopy: -

Electromagnetic radiation, microwave absorption: rotational spectra, infrared absorption: diatomic vibrational spectra, polyatomic vibrational spectra, rotational vibrational spectra, visible ultraviolet absorption: electronic spectra, nuclear spin states, nuclear resonance spectroscopy. 10 hrs

Reference Books:

1. P.W. Atkins, Physical Chemistry, 5th ed. ELBS-Oxford University Press. 1994
2. D.A. Mcquarrie and J.D. Simon, Physical Chemistry, Viva Books Pvt. Ltd New Delhi (Viva Low-priced Student Edition :South Asian Edition) Original Edition: University Science Books, California. (1998)
3. G.K. Vemulapalli, Physical Chemistr. Prentice Hall of India, New Delhi. (1997)
4. G.M. Barrow, Physical Chemistry, 5th ed., Tata McGraw-Hill, New Delhi. (1988)
5. S.K. Dogra and S. Dogra., Physical chemistry through problem. Wiley Eastern Ltd. (1993)
6. J O M Bockris and A. Reddy, Modern Electrochemistry Vol. I & II, Plenum Pub. Corp. New York (1970)
7. K.J. Laidler, Chemical Kinetics, New York: Harper and Row (1987)
8. R.P. Rastogi and R.R. Mishra, An Introduction to Chemical Thermodynamics 6th ed, Vikash Pub. House, India. (1996)
9. S.O. Pillai, Solid State Chemistry, Wiley Eastern Ltd. (1994). 531 7/P644
10. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of analysis, 6th ed, Van Nostrand (1981)
11. F. Daniels, Mathematical Preparation for Physical Chemistry, McGraw Hill Book Company,

Organic Chemistry

Course Title: Organic Chemistry
Course No.: Chem 513
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : I

Course Objectives :

- To provide basic knowledge of reaction mechanism in organic chemistry
- To give a clear idea of organic reagents in synthesis
- To give acquaintance with natural product chemistry
- To provide an idea of application of spectroscopy techniques.

Course Contents:::

Group A

Acids and Bases: Bronsted theory, acidic and basic solvents, measurement of solvent acidity (no mathematical derivation) **2 hrs.**

Acid and base catalysis (general), Lewis acids bases, hard and soft acids and bases, effects of structure on the strength of acids and bases, effect of the medium on acids and base strength **3 hrs.**

Effect of Structure on Reactivity: Resonance and field effect, steric effect, Hammett equation **3 hrs.**

Aliphatic Nucleophilic substitution: Review lecture, the neighboring - group mechanism, neighboring - group participation by pi and sigma bonds, non-classical carbocations **3 hrs.**

Aromatic Nucleophilic Substitution: Review lecture, the benzyne mechanism **2 hrs.**

Aromatic Electrophilic Substitution: Review lecture, orientation and reactivity in mono substituted benzene ring **2 hr.**

Aliphatic Electrophilic Substitution: Review lecture, bimolecular mechanism SE_2 , SE_1 and SE_i -mechanism **2 hrs.**

Addition to Carbon – Carbon multiple bond: Review lecture, addition to conjugated system, addition to cyclopropane ring **2 hrs.**

Addition to Carbon - Hetero Multiple Bond: Review lecture, mechanism and reaction **5 hrs.**

Elimination Reaction: Review lecture, brief introduction to elimination reaction, $E1cB$ mechanism, orientation of double bond **5 hrs.**

Free Radical Substitution: Review lecture, free radical mechanism in general, free radical substitution mechanism and reactions **3 hrs.**

Group B

Photochemistry: Basic concepts of photochemical energy, electronic excitation, energy transfer, quantum efficiency, photochemical reaction, photochemistry of carbonyl, compounds and olefines. **10 hrs**

Introduction to electrocyclic and cycloaddition reaction **3 hrs.**

Chemistry of Heterocyclic Compounds (Reaction and Synthesis of the Following): Three and four membered heterocycles, (aziridine, azetidine, oxiranes, thiiranes) **6 hrs.**

1,3 azoles and imidazole, oxazole and thiazole 6 hrs.
quinolines isoquinolines and indole 6 hrs.

Organometallic Compounds (Preparation and Application):

Organomagnesium, organoaluminium, Organolithium compound 2 hrs.

Synthesis by Functional Group Interconversion: 5 hrs.

Group C

Macromolecular Chemistry: Introduction, mechanism of polymerization 5 hrs.

Disaccharides (sucrose, maltose), polysaccharides (starch, cellulose) 4 hrs.

Synthesis of Small ring (3-4 membered ring) Medium sized ring (5-7) and Large ring (above 8 member) muscone, civetone 4 hrs.

Molecular Symmetry and Chirality: Introduction, symmetry operation and symmetry elements (simple or proper axis of symmetry, plane of symmetry, centre of symmetry, alternating axis of symmetry) 2 hrs.

Racemization and Methods of Resolution: Mechanism involving carbanions, carbocations, free radicals and rotation around bonds 4 hrs.

Mechanical separation, resolution through the formation of diastereomers, correlation based on asymmetric synthesis, Cram's and Prelog's rule 4 hrs.

Supramolecular Chemistry: Concepts of the language of supramolecular chemistry, examples of supramolecular compounds, Crown ether 2 hrs.

Group D

Advanced Treatment of Spectroscopic Techniques and Their Applications:

IR, UV, Mass, ^1H nmr, ^{13}C nmr) 8 hrs.

Basic Principles of solvent extraction and application in analytical chemistry 2 hrs.

Mechanism of ion exchange, Techniques of ion exchange 1 hr.

Chromatography: i) Adsorption ii) Partition iii) Gas chromatography (iv) HPLC 8 hrs.

Introduction to Natural Product Chemistry: Phytochemical screening, isolation, purification, general discussion on structure elucidation, synthesis and biosynthesis, examples from terpenes, alkaloid, flavonoids (citral, nicotine, methoxyflavanone etc) 6 hrs.

Reference Books:

1. J. D. March, *Advanced Organic Chemistry; 3rd Edition*, McGraw – Hill Book Company ✓
2. Charles Depuy, *Molecular reaction and Photo-Chemistry*; Prentice Hall ✓
3. E.L. Eliel, *Stereochemistry*; McGraw – Hill Book Company
4. D. Nasipuri, *Stereochemistry of Organic Compounds*; Wiley Eastern Ltd.
5. R.E. Ireland, *Organic Synthesis*; Prentice Hall
6. S.M Khopkar, *Basic Concept of Analytical Chemistry*; Wiley Eastern Ltd. ✓
7. K.R. Palak, *Stereochemistry*; Taleju Prakashan, Kathmandu, 1996
8. J.A. Joule and G.F. Smith, *Heterocyclic Chemistry*; Van Nostrand Reinhold Corp. ✓
9. Thomas I. Gilchrist, *Heterocyclic Chemistry*; Longman 3rd Ed. (1997)
10. I. L. Finar, *Organic Chemistry vol I and II*; ELBS ✓

- ✓ 11. Silverstein, Bassler Morrill, Spectrometric Identification of Organic Compounds; 5th edition, John Wiley and Sons Inc, (John Dyer)
- ✓ 12. Seyhan Ege, Organic Chemistry; D.C. Heath and Company ✓
- ✓ 13. G.S. Mitra, Introduction to Polymer Chemistry; Wiley Eastern Ltd. Ind. (1993)
14. Jean- Marie Lehn, Supramolecular Chemistry; VCH Weinheim 1995.

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- ✓ 11. Silverstein, Bassler Morrill, Spectrometric Identification of Organic Compounds; 5th edition, John Wiley and Sons Inc, (John Dyer)
- ✓ 12. Seyhan Ege, Organic Chemistry; D.C. Heath and Company ✓
- ✓ 13. G.S. Mitra, Introduction to Polymer Chemistry; Wiley Eastern Ltd. Ind. (1993)
14. Jean- Marie Lehn, Supramolecular Chemistry; VCH Weinheim 1995.

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Research Methodology in Chemistry

Course Title: Research Methodology in Chemistry
Course No.: Chem 514
Nature of the course: Theory

Full Marks : 50
Pass Marks : 20
The year : I

Course Objective : To impart to the students the knowhow on research methodology in chemistry.

Course Contents:

Distinctive Concept: The scientific method of research methodology and research methods. **4 hrs.**

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, different areas of chemistry e.g. theoretical, experimental, synthetical, analytical and applied **6 hrs.**

Literature Survey: How to use 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, etc., identification of research problem and proposal writing. **4 hrs.**

Tools and techniques used in Research: Tools used in spectroscopy, chromatography, chemical and physical methods, etc., solvent purification, solvent drying, reagent preparation, special Lab techniques and experimental setting., grades of reagent, cost factors, hazards due to chemicals, apparatus and reaction procedure, vacuum line techniques, handling of air sensitive compounds and hazardous chemicals , chromatographic techniques, spectroscopic techniques ,chemical techniques, high and low pressure techniques, techniques to study fast reaction, high and low temperature techniques , use of nonaqueous solvents **24 hrs.**

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, nmr, ¹³Cnmr, ms, Gc-ms and X-ray-crystallography and different chromatograms **15 hrs.**

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 **7 hrs.**

Term Paper: To be submitted by the students

References Books:

1. G.H. Jaffery etal, *Text book of Quantitative Chemical Analysis*; ELBS, Langman Group UK Ltd., 1989

2. Bates and Schaefer, Research Technique in Organic Chemistry; Printice Hall of India
3. I.L. Finar, Textbook of Practical Organic Chemistry; Longman Group Limited
4. H.J.E. Loewenthal, Guide for the Perplexed Organic Experimentalist; Heyden, London (1980)
5. Paul Stapleton, Writing Research Paper; An easy guide for non-native english speaker, ACIAR, Canberra (1990)
6. R.J. Angelici, Synthesis and Technique in Inorganic Chemistry; W.B. Saunders Company (Saunders Golden Series), Philadelphia London Toronto (1969)
7. J.D. March, Advanced organic Chemistry 3rd edition, Mc Graw Hill, Book Company
8. M.L. SHARMA (BEST BOOK)
9. Keshav Paudel (BEST BOOK) [9841502945]
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10. Amit Dhurgana (BEST BOOK)

Inorganic Chemistry (Practical)

Course Title: Inorganic Chemistry (Practical)

Course No.: Chem 515

Nature of the course: Practical

Full Marks : 50

Pass Marks : 20

The year : I

Course Objective :

- To acquaint the students with qualitative and quantitative analytical methods and
- To familiarise them with the techniques of preparation and with the characterization of co-ordination compounds.

Course Contents:

Volumetric Analysis:

- Determination of ferrous and ferric ion in a mixture by dichromate solution
- Determination of iron and copper in a mixture by dichromate solution.
- Determination of percentage purity of pyrolusite by arsenious oxide.
- Determination of copper as oxinate in CuSO_4 by using KBrO_3 .
- Determination of percentage of available chlorine in bleaching powder by using KBrO_3 .
- Determination of percentage purity of KBr by using adsorption indicator.
- Determination of amount of NaCl and KCl in a mixture by AgNO_3 .
- Determination of amount of Mn & Mg by EDTA in a mixture.
- Determination of amount of Cl^- & Br^- in mixture by AgNO_3 .
- Determination of Ca , Mg and Mn by the use of EDTA

Gravimetric Analysis:

- Estimation of Cu as thiocyanate and Zn as pyrophosphate in a mixture of the two.
- Estimation of Ca as oxide and Mg as pyrophosphate in a mixture of the two.

Salt Analysis:

- Qualitative analysis of inorganic salt mixture involving 8 radicals excluding rare earth metals by semi-micro methods.

Preparation:

- Preparation of cuprous thiourea complex.
- Preparation of sodium nitroprusside $\text{Na}_2 [\text{Fe}(\text{CN})_5 \text{NO}] \cdot 2\text{H}_2\text{O}$
- Preparation of cuprous oxide and characterization
- Preparation of about 6 to 8 complexes

Text-Books:

1. A.I. Vogel, *Qualitative Analysis*: E.L.B.S. (1994).
2. A.I. Vogel, *Quantitative Analysis*: E.L.B.S. (1994).
3. Palmer, *Experimental Inorganic Chemistry*: Cambridge University Press, UK (1954)
4. Angelici, *Synthesis & Technique in Inorganic Chemistry*: W.B. Saunders Co. (Sounders Golden Series), Philadelphia, London, Toronto (1969)

Physical Chemistry

Course Title: Physical Chemistry
Course No.: Chem 516
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : I

Course Objective : To make the students capable of conducting physical chemistry experiments and analysing the data independently.

Course Contents:

Electrochemistry

1. Conductometric titration of a mixture of weak and strong acid.
2. Conductometric titration of polybasic acid.
3. Determination of solubility and solubility product of sparingly soluble salt by conductometric method.
4. Potentiometric titration of phosphoric acid and determination of first and second dissociation constants
5. Potentiometric titration of halide mixture.
6. Potentiometric titration involving redox reaction and determination of formal potential
7. Determination of transport number by Hittorf's method
8. Verification of Nernst law of electrode potential.
9. Determination of standard electrode potential of Ag/Ag^+ electrode.
10. Determination of standard electrode potential of quinhydrone electrode.
11. Experiments involving pH-meter.
12. Investigation of antimony electrode as pH-probe.
13. Analysis with ion selective electrode.
14. Verification of Henderson law.

Chemical Kinetics

1. Determination of order of reaction for the oxidation of alcohol by dichromate by titrimetric method.
2. Kinetics of saponification of ethyl acetate by conductometric method.
3. Determination of total order of reaction between oxalic acid and chromic acid.
4. Energy of activation of acid catalyzed hydrolysis of methyl acetate.

Spectrophotometry

1. Spectrophotometric determination of chromium (VI) by 1,5 diphenyl carbzide as a reagent for colour development.

Miscellaneous

1. Determination of equilibrium constant of $\text{I}_2 + \text{KI} \rightleftharpoons \text{KI}_3$ by distribution method.
2. Determination of radius of molecules by viscosity measurements.
3. Determination of cross sectional area of COOH group by measuring the variation of surface tension with concentration of butyric acid.
4. Thermometric titration of strong acid and base.
5. Determination of R_f value of different acid base indicators and separation of indicator mixture by paper chromatography.

Reference Books:

1. M.K.Sthapit & R.R.Pradhananga, Experimental Physical Chemistry, Taleju Prakashan, Kathmandu. (1998)
2. Findlay's Practical Physical Chemistry: Longman Group Ltd., Hong Kong, Longman Inc, NY.
3. H.A. Neidig, W.J.Straton, (compiled) Modern Experiments for Introductory Chemistry [Reprint from Journal of Chemical Education] 2nd Ed IUPAC CTC by arrangement with Division of Chemical Education, Wiley Eastern Ltd, New Delhi. (1994)

Organic Chemistry Practical

Course Title: Organic Chemistry Practical
Course No.: Chem 517
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : I

Course Objective : To train the student in handling different equipments and train them further in isolation, identification and preparation of different organic compounds.

Course Contents:

1. Purification and drying of solvents and chemicals (recrystallization, vacuum distillation, fractional crystallization, fractional distillation, use of Buchner funnel, dryings of compound using drying piston, etc.) **16 hrs.**
2. An experiment on thin layer chromatography, Co TLC and preparative TLC. **12 hrs.**
3. An experiment based on paper chromatography. **8 hrs.**
4. An experiment on column chromatography. **12 hrs.**
5. Isolation of caffeine from tea. **12 hrs.**
6. Isolation of an essential oil. **12 hrs.**
7. Synthesis of two different organic compounds involving not more than two steps. **32 hrs.**
8. Identification of organic compounds such as aldehydes, ketones, acids, esters, amines, nitro compounds, amides, phenols, hydrocarbons, carbohydrates, etc. and preparation of two derivatives for each. **80 hrs.**
9. An experiment on photochemistry **8 hrs.**
10. An experiment on mixed melting points **4 hrs.**
11. An experiment on chemical kinetics (titrimetric method) **8 hrs.**
12. Construction of a manometer and its use in vacuum distillation of an organic compound **12 hrs.**
13. Determination of saponification value of an oil. **12 hrs.**
14. Purification of water through a fabricated charcoal column. **8 hrs.**
15. An experiment on molecular weight determination (Rast method). **8 hrs.**
16. Determination of iodine value of an oil. **8 hrs.**

Reference Books:

1. B.B. Dey, M.V. Sitaraman and T.R. Govindachari, *Laboratory Manual of Organic Chemistry; Third revised edition*, S. Viswanathan Publisher.
2. N.K. Vishnoi, *Advanced Practical Organic Chemistry; Second revised edition*, Vikas Publishing Pvt. Ltd.
3. A.I. Vogel, *Elementary Practical Organic Chemistry, Part 2, Second edition*
4. R.L. Shriner, R.C. Fuson and D.Y. Curtin, *The Systematic Identification of Organic Compounds - A Laboratory Manual; Fifth edition*, John Wiley & Sons, Inc.

Second Year

Inorganic Chemistry

Course Title: Inorganic Reaction Mechanism Bonding
and Structure

Course No.: Chem 611

Nature of the course: Theory

Full Marks : 100

Pass Marks : 40

The year : II

Course Objective :

- To acquaint the students with different types of inorganic reaction mechanisms;
- To provide them with knowledge on theories of bonding and structures of inorganic compounds.

Course Contents:

Inorganic Reaction Mechanism: Introduction: Kinetics and mechanism, stoichiometric mechanism and intimate mechanism, kinetic and thermodynamic properties of complexes (labile, inert, stable and unstable)

Substitution Reactions of Octahedral Complexes: Lability and d electron configuration

Mechanism for Ligand Substitution Reactions: i.) Dissociation (d) mechanism and associated (a) Mechanism ii.) Theoretical approach of substitution mechanism iii.) Nucleophilic reactivity iv.) Effect of electronic structure of central atom v.) Kinetic application of Crystal Field Theory vi.) Mechanism of substitution reaction of Complexes of Co (III)

Experimental test of mechanism : Base hydrolysis of Co (III) complexes , Acid hydrolysis , π bonding dissociation reactions of octahedral complexes Stereochemistry of octahedral substitution reactions

Substitution without breaking the metal – ligand bond, Racemization reaction
Substitution Reactions of Square Planar Complexes: substitution reactions, Extra kinetic properties of Pt (II) complexes

Trans Effect: Theories of trans effect (polarization theory, π - bonding theory, molecular orbital theory)

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 temperature Catalysis of substitution reaction by Pt (II) complexes.

Redox Reactions: 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, complimentary two equivalent exchange, electron transfer through extended bridge, crystal field effect, Marcus Theory, orbital symmetry in electron transfer, photochemical reactions ✓

Determination of Stability Constants: Overall stability constants, stepwise stability constants, importance of stability constants

40 hrs.

Activity and concentration quotients, control of activity coefficients, composition of ionic medium, limitations, stoichiometric constants, thermodynamic constants

Basic Principle: Kinetic approach, equilibrium approach, determination of (η) , calculation of free ligand concentration "a", properties involving intensive factors, The methods of continuous variation

Calculation of overall stability constants: Job's method, Bent and French's method, Yoe and Jones's method, Determination of concentration variables using competitive reactions, the system B, A, H, methods adopted by J. Bjerrum, Calvin and Wilson

20 hrs. *

Computation of stability constants from the functions $\Pi(a)$ and $\alpha_c(a)$, Experimental determination of Stability Constants.

* Spectra and Bonding of Co-ordination compounds

Ligand Field Spectra for 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 , non-crossing rule, nephelauxetic effect, Orgel, Tanabe-Sugano diagrams, correlation diagrams, Racah parameter, energy level calculations, spin orbit coupling, Spectra of d^1 - d^9 ions, spectra of second and third row transition elements, Complexes, lowering of symmetry, Effects of lowering symmetry, Charge transfer bands.

Molecular orbital description of bonding: bonding in octahedral complexes, bonding in tetrahedral complexes, quantitative calculation of $10 Dq$, 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.

Magnetic properties of complexes 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

40hrs.

Abnormal valencies: Metal ions in low and high oxidation states, Stabilization of oxidation states and π bonding, Stabilization of low oxidation states through co-ordination

20 hrs.

Text and Reference Books:

1. F. Basolo and R. Pearson, *Mechanisms of Inorganic Reactions*; Wiley, New York
2. R.B. Jordan, *Reaction Mechanisms of Inorganic and Organo Metallic Systems*; Oxford University Press, New York, 1991
3. R.G. Wilkins, *The Study of Kinetics and Mechanisms of Reactions of Transition Metal Complexes; second Ed.*, V.C.H. Publishers, 1991
4. B. Douglas, D. McDaniel, J. Alexander, *Concepts and Models of Inorganic Chemistry; third Ed.* Wiley, 1994

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5. H. Taube, *Electron Transfer Reactions of Complex Ion in Solution*; Academic Press, New York, 1970
6. C.H. Langford and H.B. Gray, *Ligand Substitution Processes*; Benjamin – Cummings, 1966
7. J.O. Edward, *Inorganic Reaction Mechanisms*; Wiley – New York
8. Francis J.C. Rossotti and Hazel Rossotti, *Determination of Stability Constants*; McGraw Hill
9. A.B.P. Lever, *Inorganic Electronic Spectroscopy; second Ed.*, Elsevier, Amsterdam, 1984
10. B.N. Figgis, *Introduction to Ligand Fields*; Interscience Publishers
11. J.K. Burdett, *Molecular Shapes*; Wiley – Interscience, New York, 1980
12. J. Lewis and R.G. Wilkins, *Modern Co-ordination Chemistry*; Interscience Publishers

5. H. Taube, *Electron Transfer Reactions of Complex Ion in Solution*; Academic Press, New York, 1970
6. C.H. Langford and H.B. Gray, *Ligand Substitution Processes*; Benjamin – Cummings, 1966
7. J.O. Edward, *Inorganic Reaction Mechanisms*; Wiley – New York
8. Francis J.C. Rossotti and Hazel Rossotti, *Determination of Stability Constants*; McGraw Hill
9. A.B.P. Lever, *Inorganic Electronic Spectroscopy; second Ed.*, Elsevier, Amsterdam, 1984
10. B.N. Figgis, *Introduction to Ligand Fields*; Interscience Publishers
11. J.K. Burdett, *Molecular Shapes*; Wiley – Interscience, New York, 1980
12. J. Lewis and R.G. Wilkins, *Modern Co-ordination Chemistry*; Interscience Publishers

Selected Topics in Inorganic Chemistry

Course Title: Selected Topics in Inorganic Chemistry
Course No.: Chem 612
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : II

Course Objectives:

- To provide knowledge of some specialized areas of inorganic chemistry and their applications;
- To provide a comprehensive idea of platinum group metals and actinide.

Course Contents:

1. Inorganic chains, cages and cluster compounds:

Cluster and cage compounds : Introduction, bonding in boranes, styx numbers, structure of boron hydrides, molecular orbital description of bonding in boron hydrides. 10 hrs.

Heteroboranes : Carboranes. 5 hrs.

Chemistry of the boranes : synthesis of boron hydrides. 5 hrs.

Cluster compounds : clusters and catalysis, molecular structure of clusters, stereochemical non-rigidity in clusters, dynamic nuclear magnetic resonance spectroscopy, electronic 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), hetero atoms in metal atom clusters, electron counting scheme for HNCC, HNCC's of the 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 PSPET MODEL, halide clusters, synthesis of metal clusters, reactivity of cluster compounds, electron precise compounds and their relation to clusters. 20 hrs.

Inorganic chains: Catenation, heterocatenation, zeolites, intercalation chemistry, one-dimensional conductors, isopolyanions, heteropolyanions 8 hrs

Lower halide and chalcogenide cluster: triangle clusters, solid-state extended arrays, compounds with M-M multiple bonds, quadruple bonds, one-dimensional solids 6 hrs.

2. Inorganic Polymers:

Introduction: addition polymerization, condensation polymerization, coordination polymerization. Homopolymers, heteropolymer, elemento organo polymer: Homosubstituted, heterosubstituted and hybrid polymers. 6 hrs.

Polymers based on boron: Homopolymers of boron (polymeric material with B-B bonds, heteropolymers of boron, Boron- Oxygen polymers, Boron-Nitrogen polymers Boron- Hydrogen polymers, Boron- Carbon polymers, Boron- Phosphorus polymers 5 hrs.

Silicon Polymers : Preparational methods, polysiloxane, silicones, Silicon-hydrogen polymers, Silicon- halogen polymers, Silicon- carbon polymers, Silicon- oxygen polymers 4 hrs.

Phosphorus polymers: condensed phosphates, cross linked phosphates, phosphorus oxygen polymers, phosphorus nitrogen polymers (phosphonitrides, phosphozenes) **3 hrs,**

Sulfur polymers: Tetra sulfur tetra nitride and related compounds sulfanes **2 hr.**

3. **Interstitial Compounds:** Classification, general chemistry and structures of carbides, nitrides, silicides, borides, **6 hrs.**

4. **Non-stoichiometric compounds:** Introduction, order and disorder of structural anomalies, structural causes of variability of composition, Classification of non-stoichiometric oxides and chalcogenides based on their composition and structure. Chalcogenides, Superconductors **8 hrs.**

5. **Alloys and Intermetallic compounds:** Introduction, methods of preparation, types of alloys, simple mixture, eutectic system, congruent system, incongruent system, solid solutions: interstitial solid solution, substitutional solid systems, phase rule application, Intermetallic compounds, Hume rothary rules: succession of Hume Rothary phases, super lattices. **7 hrs.**

6. **Chemistry of Gr. VII B (7) Technetium and Rhenium:**
Oxidation states and stereochemistry ; Important Compounds: Oxides and sulfides, halides, multiply bonded dirhenium and ditechinitium compounds, oxo compounds and complexes **4 hrs.**

7. **Chemistry of Gr. VIII The platinum group metals (Ru, Os, Rh, Ir, Pd, Pt)**
: Occurrence and general remarks on the chemistry of platinum metals important compounds, Ruthenium and Osmium Group VIII (8) Oxidation state, coordination number and geometry oxocompounds of ruthenium and osmium, halide complexes, complexes of nitrogen donor ligands, nitric oxide complexes, tertiary phosphine and related complexes, lower oxidation states, 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 (III) and Ir (III) , Complexes of Rh (II) and Ir (II), 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 **11 hrs.**

8. **The 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-amerium elements, The super heavy elements **10 hrs.**

Text and Reference Books:

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: fifth ed. John Wiley and Sons. (1988)

2. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic chemistry; 4th Ed, Harper Collins., (1993)
3. Bodie Douglas, Darl McDaniel and John Alexander, Concepts and Models of Inorganic Chemistry; third Ed, John Wiley and Sons. (1994)
4. Eds M. Zeldin, K.J. Wynne and H.R. Allcock, A.C.S. Inorganic and Organometallic Polymers; Symposium Series 360, American Chemical Society, Washington D.C. (1988).
5. J.E. Mark, H.R. Allcock and R. West, Inorganic Polymers; Prentice-Hall Englewood Cliffs N.J. (1992)
6. H.J. Emeleus and A.G. Sharpe Ed, Advances in Inorganic Chemistry and Radiochemistry, vol. 18 (K. Wade, Structural and Bonding Patterns in Cluster Chemistry); Academic press, New York 1976
7. H.J. Emeleus and A.G. Sharpe Ed., Advances in Inorganic Chemistry and Radiochemistry, vol. 18 (Robert E. Williams, Co-ordination Number; Pattern Recognition Theory of Carborane Structure); (1976).
8. H.J. Emeleus and A.G. Sharpe Ed., Advances in Inorganic Chemistry and Radiochemistry, vol. 23 (Henry Selig and Lawrence B. Ebert, Graphite Intercalation Compounds); Academic press New York 1980
9. F.G.A. Stone and W.A.G. Graham, Inorganic Polymers; Academic Press, New York.
10. D.N. Hunter, Inorganic Polymers; Blackwell Scientific Publications, Oxford
11. H.J. Emeleus and A.G. Sharpe, Modern Aspects of Inorganic Chemistry; 4th Ed. Sixth Indian Reprint Universal Book Stall, New Delhi 1992,
12. Satya Prakash, Advanced Chemistry of Rare Elements; Chemical Publishing Co., New York.
13. K.W. Bagnall, The Actinide elements; American Elsevier, Amsterdam, (1972)
14. V.I. Spitsyn and J.J. Katz Eds., The Chemistry of Transuranium Elements; Elmsford, N.Y. (1976).
15. L. Mandelcorn Ed., Non-stoichiometric compounds; Academic Press.
16. W.Hume Rothery The Structure of metals and Alloys Institute of metal London 1936.
17. D.C. Bradley, R.C. Mehrotra and D.P. Gaur Metal alkoxides; Academic Press, New York, (1978).
18. Ed. M.M. Edelstein, Actinides in Perspective; Pergamon Press, New York (1982).
19. J.J. Katz, G.t. Seaborg and L.R. Morss, The Chemistry of the Actinide Elements; second Ed. Chapman and Hall (1986).
20. M.A.K. Lodhi, Superheavy Elements; Pergamon Press, New York, (1976).
21. C.Keller, The Chemistry of Transuranium Elements; Springer Verlag (1971)
22. A.F. Wells, Structural Inorganic Chemistry; 4th Ed. Clarendon Oxford (1975).
23. A. Robenau Ed., Problem of Non-Isichiometry; North-Holland Publishing Co., Amsterdam London (1970).

Organometallics and Bio-Inorganic Chemistry

Course Title: Organometallics and Bio-Inorganic Chemistry Full Marks : 100
Course No.: Chem 613 Pass Marks : 40
Nature of the course: Theory The year : II

Course Objective :

- To give a comprehensive idea of the use of organo-metallic compounds
- To acquaint the students with basic principles of bio-inorganic chemistry

Course Contents:

1. Organometallic compounds: Introduction, classification based on the polarity of M-C bond, general characteristics of different types of organometallic compounds. **6 hrs.**

Organometallic compounds of the main group elements: stability of organometallic compounds (thermodynamic and kinetic stability), stability towards oxidation, stability towards hydrolysis. **6 hrs.**

Preparative routes for metal-carbon bond formation, factors governing formation of C-H bonds, oxidative addition, transmetallation, carbanion-halide exchange, metal-hydrogen exchange, metal-hydride-alkene addition, methylene insertion, miscellaneous methods **6 hrs.**

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 ligands

Compounds with 6 electron ligands **10 hrs.**

Fluxional organometallic compounds: Synthetic and catalytic aspects of organometallic chemistry **6 hrs.**

Use of organo lithium, organo magnesium, organometallics of Zn, Cd, Hg in synthesis, use of organo copper, use of organo palladium compounds in synthesis **10 hrs**

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 **10 hrs.**

2. Metal alkoxides: Introduction, preparative methods, properties, structural aspects of metal alkoxides (alkoxides of Al, Tl, Ti, Nb, Li, U, etc.) , Applications , Calixarenes **8 hrs.**

3. Bioinorganic Chemistry :

Essential and trace elements in biological systems **4 hrs.**

Role of alkali and alkaline earth metal ions in biological systems and their transport across the membrane (ion pumps) **4 hrs.**

Metal complexes as oxygen carriers – haemoglobin and myoglobin, non-porphyrin oxygen carriers, hemerythrin and hemocyanin, synthetic oxygen carriers 10 hrs.

Mechanism of electron transfer reaction in metal complexes, electron transfer proteins (Ferredoxins and Rubredoxins) blue copper proteins 10 hrs.

Photosynthesis: chlorophyll and the photosynthetic reaction center 6 hrs.

Metalloenzymes: carboxypeptidase, carbonic anhydrase oxidases, vitamin B₁₂ and the B₁₂ coenzymes 10 hrs.

Biochemistry of iron metal complexes (ferritin, transferrin, siderophores) for storage and transfer 4 hrs.

Toxicity of metals, metal complexes as drugs and anti-cancer agents 4 hrs.

4. **Peroxide and Peroxides:** General methods of preparation, chromium peroxides, peroxyacids of chromium, molybdenum and tungsten, perbromic acid, pernitric acid, peroxy compounds of cobalt 6 hrs.

Reference Books:

1. G.E. Coates, M.L.H. Green, P. Powell and K. Wade, *Principles of Organometallic Chemistry*; Chapman and Hall, London (1977).
 2. I. Haiduc and J.J. Zuckermann, *Basic Organometallic Chemistry*; Walter de Gruyter, N Y, (1985).
 3. G. Wilkinson, F.G.A. Stone and E.W. Abel (Eds.), *Comprehensive Organometallic Chemistry*; Pergamon Press, New York, (1982).
 4. C. Masters, *Homogenous Transition Metal Catalysis*; Chapman and Hall, London, (1981).
 5. J.P. Collman, L.S. Hegeudus, J.R. Norton and R.G. Finke, *Principles and Applications of Organotransition Metal Chemistry*; University Science Books, California (1987).
 6. R.C. Mehrotra and A. Singh, *Organometallic Chemistry (A Unified Approach)*; Wiley Eastern Limited (1992).
 7. F.A. Cotton, G. Wilkinson and P.L. Gaus, *Basic Inorganic Chemistry: third Ed.*; John Wiley and Sons, (1995).
 8. J.E. Huheey, E.A. Keiter and R.L. Keiter, *Inorganic Chemistry: 4th Ed.* Harper-Collins, (1993).
 9. F.A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry: 5th Ed.* John Wiley and Sons, (1988).
 10. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Model of Inorganic Chemistry; 3rd Ed* John Wiley and Sons, (1994).
 11. I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine Eds., *Bio-Inorganic Chemistry*; University Science Books, Mill Valley, CA, (1994).
 12. S.J. Lippard and J.M. Berg, *Principles of Bioinorganic Chemistry*; University Science Books, Mill Valley CA (1994).
 13. J.R.F. da Silva, R.J.P. Williams, *The Biological Chemistry of the Elements – The Inorganic Chemistry of Life*; Clarendon Press, Oxford (1991).
- Relevant articles from *Progress in Inorganic Chemistry*, *Advances in Organometallic Chemistry* will be used.

Inorganic Chemistry (Practical)-I

Course Title: Inorganic Chemistry (Practical)-I
Course No.: Chem 614
Nature of the course: Practical

Full-Marks : 75
Pass Marks : 30
The year : II

Course Objective :

- To acquaint the students with various techniques of qualitative and quantitative analysis
- To acquaint the students with techniques for the preparation and characterization of inorganic complexes

Course Contents:

Volumetric Analysis

Determination of ferrous and ferric ion in a mixture by ferric salt.

Determination of copper & cadmium in mixture volumetrically & gravimetrically.

Determination of Mn, Mg and Zn in a mixture using EDTA.

Analysis of a low melting Bi-Pb-Cd-Sn alloy by EDTA.

Salt Analysis

Qualitative analysis of salt mixture involving 8 radicals including rare earth metals and interfering radicals by semi- micro method.

Preparation

Preparation of trioxalato ferrate and estimation of percentage of oxalate and iron in the prepared sample. Compare the IR spectrum with potassium oxalate or oxalic acid. Determine the molar conductivity.

Preparation of hexamine cobalt chloride and estimate the percentage of cobalt in prepared sample. Compare IR with ammonium salt. Determine the molar conductivity.

Preparation of cuprous-mercuric iodide $[\text{Cu}_2\text{HgI}_4]$.

Gravimetric Analysis

Any four alloys, dolomite and cement.

Inorganic Chemistry (Practical) - II

Course Title: Inorganic Chemistry (Practical) - II
Course No.: Chem 615
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : II

Course Objectives:

- 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 work;
- To familiarise them with making use of some instruments.

Course Contents:

Salt Analysis: - Spot test.

Preparation

Preparation of trans $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$ and study of its isomerism by electronic spectroscopy.

Preparation of meridonal and facial $[\text{Co}(\text{NH}_3)_3(\text{NO})_3]$.

Preparation of nitrate pentammine cobaltic (III) nitrate $[\text{Co}(\text{NH}_3)_5(\text{NO}_3)](\text{NO}_3)_2$ from aqua pentaammino cobalt oxalate

$[\text{Co}(\text{NH}_3)_5(\text{H}_2\text{O})_3]_2(\text{C}_2\text{O}_4)_3$ and estimation of oxalate.

Preparation of ferrocene and its acetylation, chromatography of ferrocene derivative

Instrumental

Determination of stability constant

Complex ion composition by Job's method

Estimation of Na, K and Ca in soil sample by flame photometry.

Estimation of iron in a sample of tomato juice spectrophotometrically.

Qualitative analysis of inorganic cations of Gr. I, II, III and IV and anions by paper chromatography.

Gravimetric Analysis: Any one alloy.

Inorganic Dissertation

Course Title: Inorganic Dissertation
Course No.: Chem 616
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : II

Course Objective :

- To make the students familiar with research works in inorganic chemistry and related fields.

Course Contents:

Research work on a topics provided by the supervisor

Quantum Mechanics and Statistical Mechanics

Physical Chemistry

Course Title: Quantum Mechanics and Statistical Mechanics Full Marks : 100
Course No.: Chem 621 Pass Marks : 40
Nature of the course: Theory The year : II

Course Objective :

- To make the students familiar with modern advances in quantum mechanics and statistical mechanics.

Course Contents:

Group A

Quantum Mechanics:

Schrödinger Equation and Particle in a Box: Schrödinger equation and wave function, linear operators, eigen value, wave function and probability, particle in one dimensional box, tunneling phenomena, Heisenberg's uncertainty principle, particle in three dimensional box. 10 hrs.

Some Postulates and General Principles of Quantum Mechanics.: Postulates of quantum mechanics, time dependent Schrodinger equation, quantum mechanical operators, virial theorem. 8 hrs

Angular Momentum: Orbital angular momentum operators, step down and step up operators for angular momentum, eigen values and eigen functions of angular momentum operators. 10 hrs.

Harmonic Oscillator and Rigid Rotator: Harmonic oscillator, energy levels of a quantum mechanical harmonic oscillator, Hermite polynomials, Legendre polynomials, rigid rotator, energy levels of a rigid rotator, rigid rotator as a model for diatomic molecule. 10 hrs

Hydrogen Atom.: Schrödinger equation for hydrogen atom, spherical harmonics, angular momentum, quantum numbers, s and p orbitals, Schrödinger equation for helium atom. 10 hrs

Approximation method: Variation methods, trial functions, secular determinant, perturbation theory. 10 hrs

Multielectron atoms: Atomic units, calculation of energy of He atom by perturbation and variation method, Hartree-Fock - Self consistent field method, spin angular momentum, antisymmetrical wave function and Slater determinant, term symbols, Hund's rule. 10 hrs

Group B

Statistical Mechanics:

Review of Basic Statistical Mechanics: Phase space, ensemble, Liouville theorem, equal priori probability, micro canonical ensemble, quantization of phase space, classical limit, various distributions using microcanonical ensemble, entropy, Gibbs paradox, Sackur-Tetrode equation, canonical and grand canonical ensemble, equipartition of energy, ideal gas in grand canonical ensemble. 18 hrs.

Partition Functions: Rotational, vibrational and translational partition functions, application of partition functions to specific heat of ideal gas, solid, and chemical equilibrium **17 hrs.**

Quantum Statistics: Bose-Einstein distribution, Bose-Einstein condensation, thermodynamic properties of ideal Bose-Einstein gas, Fermi-Dirac distribution, degenerate Fermi gas, comparison of Bose-Einstein, Fermi-Dirac and Maxwell-Boltzmann statistics, application of quantum statistics, electrons in metals, magnetic susceptibility of free electrons. **17 hrs**

Reference Books:

1. F.L.Pilar, *Elementary Quantum Chemistry*, McGraw Hill Book Co. New York.
2. D.A.Mcquarrie and J.D.Simon, *Physical Chemistry*, Viva Books Pvt.Ltd New Delhi (Viva Low-priced Student Edition :South Asian Edition) Original Edition: University Science Books, California. (1998)
3. A.K.Chandra *Quantum Chemistry*, Tata McGraw Hill (1994)
4. D.A.Mcquarrie, *Quantum Chemistry*, University Science Books, Mill Valley. (1983)
5. S.Glasstone., *Theoretical Chemistry*, Mac Millan and Co Ltd, st Martin's street London
6. B.K.Agrawal and M.Eisner, *Statistical Mechanics*, Wiley Eastern. ..(1988)
7. D.A.Mcquarrie, *Statistical Mechanics*, Harper Row. (1976)

Electrochemistry and Solid State Chemistry

Course Title: Electrochemistry and Solid State Chemistry
Course No.: Chem 622
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : II

Course Objective :

To provide the students with the knowledge of development in modern electrochemistry and solid state chemistry.

Course Contents:

Group A

Advanced Electrochemistry :

Electrified Interface: Thermodynamics of electrified interface, structure of double layer at metal electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern Models, relative contributions of Helmholtz-Perrin and Gouy-Chapman capacities, electrocapillary phenomenon, structure of semiconductor electrolyte interface, semiconductor electrodes, photoeffects at semiconductor electrodes, photoelectrochemical cells. **20 hrs.**

Electrode kinetics: Butler-Volmer equation, exchange current, drift current, overpotentials, low field and high field approximations, polarizable and non-polarizable interfaces, Nernst equation, multistep electrode reaction, determination of mechanism of multistep electrode reaction, mass transfer to electrode surface. **20 hrs.**

Some electrochemical system of technological interest: Electrochemical theories of corrosion, corrosion current and corrosion potential, example of corrosion, corrosion prevention, passivation, mechanism of passivation, electrochemical energy conversion : Fuel cells and batteries, energy density, primary and secondary batteries, electrocatalysis, electrodeposition on metals, electrocrystallization. **20 hrs.**

Modern electrochemical technique: Design of electrochemical cells (working, reference and counter electrodes) potential step methods, potential sweep methods including cyclic voltametry, Tafel plots and its applications, rotating disk electrode. **10 hrs.**

Group B

Solid state

Bonding in solids: Empirical classification of crystal binding, ionic crystals, covalent crystals, metallic crystals, molecular crystals, hydrogen bonded crystals, Ionic bonding: Lattice energy of ionic crystals, lattice energy of sodium chloride, evaluation of Madelung constant, calculation of repulsive potential exponent from compressibility data, Born-Haber cycle, factor affecting crystal structures. **10 hrs.**

Electrical properties of metals: Quantum mechanical theory of free electrons, origin of band gap, effect of Fermi-Dirac distribution on the electrical conductivity, density of states and Fermi energy. Fermi distribution function, band theory of solids, electrons in periodic field of crystal (Kronig-Penney)

Model), Brillouin zones, distinction between metals, insulator and semiconductors. 10 hrs. 3.

Imperfections in solids: Defects in solids, concentration of point defects: vacancy in metals, Schottky defects in ionic solids, Frenkel defects in ionic solid, specific defects: impurities in metals, vacancy through alio-valent impurities in ionic solids, charge compensation in ionic solids, non-stoichiometry, colour centres. 10 hrs. 2

Solid state reactions and crystal growth: Wagner's theory, oxidation of metals, kinetics of oxide film growth, sintering, photographic process, techniques of crystal growth and purification : zone refining, crystal growth from solutions, growth from melt, vapour deposition technique. 10 hrs. 1

Superconductivity: Occurrence of superconductivity, conventional and organic superconductors, fullerenes, high temperature superconductors, and applications of superconductors. 10 hrs. 5

Reference Books:

Electrochemistry

1. J O M Bockris and A.Reddy, Modern Electrochemistry Vol. I & II , Plenum Pub. Corp. NY 1970
2. Allen J, Bard and Larry R. Faulkner., Electrochemical Methods , John Wiley, New York 1980
3. E.Gileadi, E.kirowa-Eisner and J Penciner. Interfacial Electrochemistry , Addison-Wesley Pub.Reading.1975
4. J.O' M.Bockris, N.Bonociocat and F.Gutmann., An Introduction to Electrochemical Science, Wykeham Pub.London 1974.

Solid state

1. D.K.Chakrabarty, Solid State Chemistry, New Age Int. Ltd. New Delhi. (1996)
2. C.Kittel, Introduction to Solid State Physics , 5th Ed. John Wiley Estern (1976) 531-652
3. H.V.Keer, Principles of the Solid State, Wiley Eastern LTd. New Delhi. (1993) 41.044, 1K256
4. S.O.Pillai, Solid State Physics, Wiley Eastern Ltd. New Delhi (1994) 31.71, 64
5. N.B.Hannay, Solid State Chemistry, Prentice-Hall of India Pvt.Ltd, New Delhi. (1976)

Alkins 541/A+52P

Barrow T/541/B 279P

Spectroscopy, Surface Chemistry and Group Theory

Course Title: Spectroscopy, Surface Chemistry
and Group Theory

Course No.: Chem 623

Nature of the course: Theory

Full Marks : 100

Pass Marks : 40

The year : II

Course Objective :

- To provide the students with advanced knowledge on Spectroscopy, surface chemistry and group theory.

Course Contents:

Group A

Surface Chemistry :

Adsorption Isotherm and Catalysis.: Failure of the Langmuir model; factors influencing the variation of the heat of adsorption with coverage, BET isotherm and multilayer physical adsorption, determination of surface area from adsorption data, Harkin-Jura, Langmuir-Hinshelwood adsorption isotherm, application of isotherm equations to adsorption, molecular sieve effect, surface catalyzed reactions, rate law from Langmuir isotherm, reaction between H_2 and N_2 .

20 hrs

Solid Surface.: Surface forces: forces of physical adsorption, energy of chemisorption, surface structure - LEED, surface composition - ESCA, 15 hrs

Group theory

Symmetry elements, symmetry operations as group elements, representation of symmetry, operations by matrices, reducible and irreducible representations, character table, properties of character tables, and reduction formula, systematic classification of molecules into point group, bond vectors and mathematical functions as bases for representations, application of group theory in chemical bonding and molecular spectroscopy.

25 hrs.

Group B

Spectroscopy:

Pure Rotational Spectra: Quantum mechanical results on rigid rotator, classification of molecules according to their moment of inertia, rotational energy levels, calculation of rotational energy levels of molecules, stark effect, selection rules and rotational spectra of symmetric top and asymmetric top molecules.

15 hrs.

Vibrational Spectra.: Simple harmonic oscillator model, vibrational energies of diatomic molecules, zero-point energy, force constant and bond strength, calculation of bond lengths and effects of isotopic substitution on diatomic molecules, dissociation energies, anharmonic oscillator, diatomic vibrating rotator, vibration of poly-atomic molecules, overtones and hot bands, P, Q and R branches, application of vibration spectra in elucidation of molecular structure from vibrational frequencies.

15 hrs

Raman spectroscopy: Quantum and classical theories of Raman effect, pure rotational Raman spectra: linear, 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 infra red spectroscopy.

10 hrs.

Electronic spectra: Frank-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model (particle in a box)

10 hrs.

Lasers, Laser Spectroscopy and Photochemistry: Components of laser, high resolution laser spectroscopy, pulsed laser and dynamics of photochemical processes.

10 hrs.

Reference Books:

1. C.N.Banwell and E.M.McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata McGraw Hill. (1994)
2. D.K.Chakrabarty, Solid State Chemistry, New Age Int.Ltd, New Delhi. (1996)
3. D.A.Mcquarrie and L.D.Simon, Physical Chemistry, Viva Books Pvt.Ltd.New Delhi (Viva Low-priced Student Edition :South Asian Edition) Original Edition: University Science Books, California. (1998)
4. G.Hertzberg, Spectra of Diatomic Molecules, Van Nostrand, New York (1950)
5. G.K. Vemulapalli, Physical Chemistry, Prentice Hall of India, New Delhi. (1997)
6. F.A.Cotton, Chemical Applications of Group Theory, Third Ed. Wiley, New York, (1990)

Physical Chemistry Practical - I

Course Title: Physical Chemistry Practical - I
Course No.: Chem 624
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : II

Course Objective :

- To acquaint the students with various experimental techniques.

Course Contents:

Compulsory Course

- 1 Verification of Debye Huckel Onsagar equation.
- 2 Experiments involving pH-meter.
- 3 Determination of acid content in squash.
- 4 Determination of nicotine content in cigarette by non-aqueous potentiometric and conductometric titrations
- 5 Study of kinetics iodination of acetone by colorimetric method.
- 6 Influence of ionic strength on kinetics of a reaction.
- 7 Determination of sodium in tap water
- 8 Determination of ammonia – N, nitrite –N and nitrate-N in water by spectrophotometric method.
- 9 Determination of iron in tomato by spectrophotometric method.
- 10 Determination of molecular weight of polymer by viscometer.
- 11 Determination of CMC of some soap by surface tension measurement.
- 12 Determination of surface area by adsorption method.

Reference Books:

- 1 M.K.Sthapit & R.R.Pradhananga, Experimental Physical Chemistry, Taleju Prakashan, Kathmandu. (1998)
- 2 B.P. Levitt Ed. Findlay's Practical Physical Chemistry, 9th revised Ed. Longman, London (1985)
- 3 H.A. Neidig, W.J.Straton (compiled), Modern Experiments for Introductory Chemistry [Reprint from Journal of Chemical Education] 2nd Ed, IUPAC CTC by arrangement with Division of Chemical Education, Wiley Eastern Ltd, New Delhi. (1994)

Physical Chemistry Practical-II

Course Title: Physical Chemistry Practical-II
Course No.: Chem 615
Nature of the course: Practical

Full Marks : 75
Pass Marks : 30
The year : II

Course Objective :

- To acquaint the students with advanced experimental techniques.

Elective Practical Course or Dissertation

Course Contents:

Electrochemistry

- 1 Analysis of a mixture of HCl, NaCl and NH_4Cl solution conductometrically.
- 2 Investigation of antimony electrode as pH-probe.
- 3 Analysis with ion selective electrode.
- 4 Construction of Silver/ silver chloride reference electrode and determination of its electrode potential.
- 5 Construction, characterization and use of precipitate base ion selective electrode.
- 6 Determination of phosphoric acid in cola soft drink.
- 7 Determination of decomposition and half wave potentials of different metal ions.
- 8 Determination of different metal ions by polarographic method.
- 9 Non-aqueous potentiometric titration to determine weak base..

Chemical Kinetics

Kinetics of catalytic decomposition of H_2O_2
Study of kinetics of inversion of sugar by polarimeter.
Determination of activation energy for the reaction between potassium persulphate and iodide with and without catalyst.

Flame Photometry

Determination of sodium and potassium in tomato/ oral hydration powder (Jeevan Jal)
Determination of calcium in vegetables/soil.

Spectrophotometry

Dissociation constant of indicator by spectrophotometer.
Determination of stability constant of complex by spectrophotometer.

Miscellaneous

Determination of cross sectional area of COOH group by measuring the variation of surface tension with concentration of butyric acid.

Use of TLC.

Separation by Column chromatography and ion exchange chromatography.
Experiments on gas chromatography.
Experiments on the use of Refractometer.
Determination of CEC of clay, zeolite, silica gel, activated charcoal etc.
Construction of phase diagram of binary system

Any other experiments introduced in class work during the year

Reference Books:

- 1 M.K.Sthapit & R.R.Pradhananga, Experimental Physical Chemistry, Taleju Prakashan, Kathmandu. (1998)
- 2 B.P. Levitt Ed. Findlay's Practical Physical Chemistry, 9th revised Ed. Longman, London (1985)
- 3 H.A. Neidig, W.J.Straton (compiled), Modern Experiments for Introductory Chemistry [Reprint from Journal of Chemical Education] 2nd Ed, IUPAC CTC by arrangement with Division of Chemical Education, Wiley Eastern Ltd, New Delhi. (1994)

Physical Dissertation

Course Title: Physical Dissertation

Course No.: Chem 616

Nature of the course: Practical

Full Marks : 50

Pass Marks : 20

The year : II

Course Objective :

- To make the students familiar with research works in physical chemistry and related fields.

Course Contents:

Research work on a topics provided by the supervisor

Organic Synthesis

Organic Chemistry

Course Title: Organic Synthesis
Course No.: Chem 631
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : II

Course Objective : To enable the students to master the skill in synthetic designs, developed so far in the field of organic chemistry.

Course Contents:

Group A

Organic synthesis (definition, history, role); 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) **15 hrs.**

Synthetic tools and reagents; synthetic planning and synthetic design; the cardinal principles of synthesis, synthetic process and steps in synthesis; carbon framework construction and functional group modification; key intermediates; starting materials; linear and convergent approach; relay approach, blocking groups, protecting groups, masking groups. **15 hrs.**

Group B

Modern synthetic concepts; retrosynthetic analysis and disconnection; retrons and transforms; strategic bonds and special sub-structures, stereo-consideration, potential symmetry, scope and limitation of synthetic tool; synthons; umpolung, control elements (equivalent, modified, region-specific and stereospecific); factors affecting the choice of a synthetic strategy. **20 hrs.**

Group C

Extensive study and application of the following synthetic reactions:

- Carbon to carbon and carbon to hetero atom bond forming reactions
- Oxidation and reduction
- Halogenation and alkylation
- Acylation, aldol condensation and related reactions **20 hrs.**

Group D

Case study of synthetic problematic examples with respect to (a) carbon skeleton, (b) stereochemistry, (c) logistics and (d) stereochemistry **7 hrs.**

Critical study of the synthesis of the following:

- | | |
|--|-------------------------------------|
| a. Tropine | b. Cholesterol ✓ |
| c. Longifolene ✓ | d. Penicillin ✗ |
| e. Prostaglandin E ₁ and E ₂ ✓ | f. Juvenile hormone ✓ 15 hrs |

Group E

Synthetic dyes; colour and constitution; synthetic drugs and chemotherapy; synthetic and semi-synthetic antibiotics; synthetic hormones. **10 hrs.**

Synthetic polymers, synthetic fibres; synthetic plastics and resins; synthetic rubber; silicones. **8 hrs.**

Synthetic uses of organometallic compounds of boron, silicon, selenium, aluminum lithium, magnesium, copper and other transition metals. **10 hrs.**

Refernce Books:

1. Robert E. Organic Synthesis; Ireland, Prentic Hall
2. Stephen Turner Principles of Synthetic Design; Elsevier Sci. Pub. Comp, NK
3. E.J. Corey, General Methods of Synthesis; Harvard University, USA.
4. Stephen Hamessian Total Synthesis of Natural Products; Chiron Approach, Pregmon Press, Oxford, 1983
- 5. H. Nozaki Current Trends in Organic Synthesis; Topics in Current Chemistry; Spring Verlag, Germany
6. H.O. House Modern Synthetic Reactions; W.A. Bezamin, New York.
7. Ian Fleming Selected Organic Synthesis; John Wiley and Sons, NK
8. K.C. Nicolaou and E.J. Sorensen Classics in Total Synthesis; VCH Germany (1996)
- ✓ 9. Anthoxy J. Chichester Organometallic Compounds; Person, John Willey (1985)
- ✓ 10. J.H. Swan and D. St. C. Black, Organometallics in Organic Synthesis; London, Chapman and Hall (1985)
- 5472
N787p 11. Richard Norman and James M. Coxon, Principles of Organic Synthesis; Blabie Academic 1993
12. H. Waldmann: Organic Synthesis Highlights, VCH, Germany (1995)
13. D.P. Curran, N.A. Porter and B. Giese : StereoChemistry of Radical reactions- Concept, Guideline and Synthetic Applications, VCH, Germany (1994)
14. J. Fahrhop and G. Penzlin ; Organic Synthesis, VCH, Germany (1994)
15. N. Anand, J.S. Bindra and S. Ranganathan, Art in Organic Synthesis; Holden-Day, San Francisco 1970
- ✓ 16. T.W. Greene: Protective Groups in Organic Synthesis, John Wiley, New York 1981

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Organic Reaction Mechanism

Course Title: Organic Reaction Mechanism
Course No.: Chem 632
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : II

Course Objective : To acquaint the students with different types of reaction mechanisms encountered in organic chemistry.

Course Contents:

Group A

Aliphatic nucleophilic substitution: Introduction and review, ion-pairs in the S_N1 mechanism, mixed S_N1 and S_N2 reactions, allylic rearrangements, nucleophilic substitution at an aliphatic trigonal carbon, nucleophilic substitution at a vinylic carbon, reactivity – the effect of substrate structure, the effect of attacking nucleophile, the effect of the leaving group, the effect of reaction medium, ambident nucleophiles – regioselectivity, eight mechanisms of ester hydrolysis, typical reactions with mechanisms **14 hrs.**

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 **8 hrs.**

Group B

Aromatic electrophilic substitution: Review, the ortho/para ratio, Ipso attack, 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 **10 hrs**

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 **5 hrs.**

Free radical substitution: Review, mechanisms at an aromatic substrate, neighboring group assistance in free radical reactions, reactivity for aliphatic substrate, reactivity in aromatic substrate, reactivity in the attacking radical, the effect of solvent on reactivity, typical reactions with mechanisms **(7 hrs.)**

Group C

Addition to carbon – carbon multiple bonds: Review, orientation and reactivity – reactivity, orientation, stereochemical orientation, typical reactions with mechanisms **8 hrs.**

Addition to carbon – hetero multiple bonds: Review, mechanism and reactivity, typical reactions with mechanisms **5 hrs.**

Eliminations: Review, the E_2C mechanism, the E_1 - E_2 - E_1CB 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, typical reactions with mechanisms **10 hrs.**

Group D

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

8 hrs.

Reactive intermediates: Carbenes – generation from α - elimination, photolysis and thermal decomposition of diazo compounds, Bamford Stevens reaction, Seyferth and coworker's method, trihalocarbonyl reaction, pyrolysis 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

8 hrs.

Nitrenes: Generation- direct photolysis, α - elimination, thermal decomposition, stereospecific and nonstereospecific reactions, insertion reaction, problems

5 hrs.

Ylids and related chemistry: Generation of phosphonium methylides, phosphonate carbanion and their reaction, generation of 1, 3- dithiane carbanions and their reactions, generation of sulfonium and sulfoxonium methylene and their reactions, problems

6 hrs.

Group E

Conservation of orbital symmetry: Electrocyclic reactions, stereochemistry of electrocyclic reactions, symmetry properties of molecular orbitals, symmetry control of electrocyclic reactions, sigmatropic reactions, examples of the stereochemistry of sigmatropic reactions, an alternate qualitative molecular orbital approach, problems

10 hrs.

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, problems

10 hrs.

Reference Books:

1. J. March, Advanced Organic Chemistry; Fourth Edition, Wiley Eastern Limited, 1992
2. Charles H. DePuy and Orville S. Chapman, Molecular Reactions and Photochemistry; Prentice-Hall of India Pvt. Ltd., 1975
3. E.S. Gould, Holt, Rinehart and Winston, Mechanism and Structure in Organic Chemistry; Holt, Reinhart and Winstron (1963)
4. Breslow : Organic Reactions Mechanism; W. A. Benjamin NY.
5. M. Jones and R.A. Moss Reactive Intermediates; Academic Press NK
6. Woodward and Hoffmann Conservation of Orbital symmetry; Verlag Chemie GmbH.
7. Peter Sykes Mechanism of Organic Reactions; Orient Longman
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
11. H.O. House, Modern Synthetic Reactions; W. A. Benjamin NY 1972
12. T.C. Bruice and S.T. Benkovic : Bioorganic Mechanism, W. A. Benjamin NY.
13. C.J. Timmous : Modern Reactions in Organic Synthesis, Reinhold, London 1970
14. E.T. Corey : The Logic Of Chemical Synthesis, John Wiley and Sons NK 1989
15. W. Appolzer : Comprehensive Organic Synthesis, B.M Trost, and Fleming I (Eds.) Perguman Press, NK 1991

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Stereochemistry and spectroscopy

Course Title: Stereochemistry and spectroscopy
Course No.: Chem 633
Nature of the course: Theory

Full Marks : 100
Pass Marks : 40
The year : II

Course Objectives :

- . To provide a panoramic view of the stereochemistry of various organic compounds;
- . To provide the knowledge on spectroscopic methods in structure elucidation.

Course Contents:

Group A

Structure and symmetry: symmetry elements σ , C_n , C_∞ , C_2 , reflection symmetry, point groups, classification of symmetry elements- No reflection symmetry (dissymmetry) and reflection symmetry, conformations without reflection symmetry (C_1 , D_n , C_2 , C_3 , D_2 , D_3), conformations with reflection symmetry (C_s , S_n , C_{2v} , C_{3v} , $C_{\infty v}$, C_{2h} , d_{2h} , d_{3h} , D_{6h} , $D_{\infty h}$, T_d , O_h and I_h)

8 hrs.

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

6 hrs.

The nature of racemates, properties of racemates (m.p., solubility, vapour pressure), determination of enantiomer and diastereomer composition (isotope dilution method, kinetic method)

5 hrs.

Racemization process (thermal method); racemization via stable achiral intermediates, excited states and free radicals), acid catalyzed and base catalyzed processes, racemization of amino acids,

Resolution: Chemical separation of enantiomers via diastereomers (tartaric acid resolution, resolution of α , β -unsaturated ketones, optical activation of menthone), asymmetric transformations of diastereomers, general methods for the separation of diastereomers, kinetic resolution, enzymatic resolution

8 hrs.

Group B

Determination of configuration of cis- trans isomers (chemical methods, physical methods), interconversion of cis- trans isomers (photochemical isomerization, directed cis- trans interconversion)

6 hrs.

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

6 hrs.

Configuration and Conformation of cyclic molecules: stereoisomerism and configurational nomenclature of ring compounds, determination of configuration of substituted 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, conformation and reactivity in cyclohexanes, chemistry of three and four membered rings, rings larger than six membered, concept of i-strain **8 hrs.**

Stereochemistry of fused rings (hydrindane, decalins, perhydrophanethrene and perhydroanthracenes), bridged rings, Bredt's rule and bridge head alkenes, paddlanes and propellanes, atenanes, rotananes, knots and Möbius strips, synthesis of cubane, adamantane, tetrahedrane, dodecahedrane and Buckminster fullerene **6 hrs.**

Group C

Stereoselective synthesis: diastereoselective synthesis of achiral compounds (cyclohexanes, stereocontrolled synthesis of E- alkene derivative via alkenes and (E,E) farnesol), 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) **10 hrs.**

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) **5 hrs.**

Chirality in molecules devoid of chiral centers: Introduction and nomenclature, allenes, synthesis of optically active allenes, determination of configuration, cyclic allenes, alkylidene cyclohexanes, 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) **8 hrs.**

Group D

Mass spectrometry: Introduction, instrumentation, determination of molecular formula, recognition of molecular ion peak, fragmentation and rearrangements, problem solving **5 hrs.**

Infrared spectroscopy: Introduction, theory , instrumentation, sample handling, interpretation of spectra and hydrogen bonding, characteristic group absorption of organic molecules, problem solving **8 hrs.**

Ultraviolet spectroscopy: Introduction, theory, sample handling, characteristic absorption of organic compounds, chromophores, auxochromes, bathochromic shift and hypsochromic shift, rules for predicting the position of absorption of homo- and heteroannular systems, problem solving **8 hrs.**

Group E

Proton magnetic resonance spectroscopy: Introduction, instrumentation, sample handling, chemical shift, simple spin coupling, protons on heteroatoms, coupling of protons to other nuclei, chemical shift equivalence and magnetic equivalence, AMX, ABX and ABC systems with the coupling constants, strongly and weakly coupled spin systems, effect of a chiral center, vicinal and geminal coupling in rigid systems, spin coupling and shift reagents
8 hrs.

^{13}C NMR spectroscopy: Introduction, peak assignments, off-resonance decoupling, chemical shifts, chemical shift equivalence, spin coupling, problem solving
8 hrs.

New dimensions in NMR: Introduction, ^1H - ^1H connectivity, spin decoupling (1-D), homo J- resolved ^1H - ^1H spectroscopy, correlated spectroscopy (COSY), ^1H - ^{13}C connectivity, J- resolved ^1H - ^{13}C spectroscopy (HET 2DJ) (2D), heteronuclear chemical shift correlation (HET COR), ^{13}C - ^{13}C connectivity, NOE difference spectrum (1- D) and the NOESY (Nuclear Overhauser and Exchange Spectroscopy) (2-D), problem solving
7 hrs.

Reference Books:

1. E.L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic compounds; John Wiley & Sons, Inc., 1994
- 16
255
2. E.L. Eliel Stereochemistry of Carbon Compounds; McGraw - Hill Book Comp. Inc
3. K. Mislow, Introduction to Stereochemistry; W.A. Benjamin Inc, 1966
- 6
91
4. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic Compounds; John Wiley & Sons, Inc., Fifth edition, 1991
- 5
5. John R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds; Prentice-Hall, Inc., 1965
6. M. Nógrádi, Stereoselective Synthesis; VCH Publishers, 1995
7. I.L. Finar Organic Chemistry; vol I and II; ELBS 1980
8. Atta Ur Rahmann : Nuclear Magnetic Resonance, Basic Principles, Springre Verlag, YK (1986)

Organic Chemistry Practical - I

Course Title: Organic Chemistry Practical - I
Course No.: Chem 634
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : II

Course Objective : To give practical training involving various techniques.

Course Contents:

1. Separation of organic mixtures based on solubility (at least 2 mixtures) **24 hrs.**
2. Synthesis of organic compounds involving three steps and their characterization by IR, UV and NMR techniques **28 hrs.**
3. Determination of the percentage purity of sugar **12 hrs.**
4. Determination of the hydroxyl group **8 hrs.**
5. Determination of specific rotation to study the inversion of cane sugar **8 hrs.**
6. An experiment based on chemical kinetics by spectrophotometric techniques **8 hrs.**
7. Phytochemical screening for alkaloids, terpenes and flavonoids **12 hrs.**
8. Determination of vitamin C in fruit juice **8 hrs.**
9. An experiment based on the use of Soxhlet extraction **8 hrs.**

Organic Chemistry Practical - II

Course Title: Organic Chemistry Practical - II
Course No.: Chem 635
Nature of the course: Practical

Full Marks : 75
Pass Marks : 30
The year : II

Course Objective : To equip the students with the techniques of separation, isolation and identification of organic compounds as well as with the technique of handling various types of equipments.

Course Contents:

1. Separation of the following organic mixture (solid-solid, solid-liquid and liquid-liquid) based on solubility involving the following reagents (10% aq. solution of NaHCO_3 , NaOH and HCl) as well as with water or ether or saturated solution of NaHSO_3 . Purification of the separated compounds is essential and is to be checked TLC and m.p. determination. **48 hrs.**
2. Synthesis of organic compounds involving not more than three steps and their characterization by IR, UV and NMR techniques. **28 hrs.**
3. An experiment on ion-exchange chromatography. **8 hrs.**
4. An experiment on gas-liquid chromatography. **8 hrs.**
5. An experiment using flame photometer **4 hrs.**
6. Determination of amino group. **8 hrs.**
7. Determination of methoxy group. **12 hrs.**
8. Estimation of nitrogen by Kjeldahl's method **16 hrs.**
9. Determination of sulphur by gravimetric method. **24 hrs.**
10. Determination of protein in milk by titration method. **8 hrs.**
11. Use of Abbe's refractometer to determine the atomic refractivities. **4 hrs.**

Reference Books:

1. B.B. Dey, M.V. Sitaraman and T.R. Govindachari, *Laboratory Manual of Organic Chemistry; Third revised edition*, S.Viswanathan publisher.
2. N.K. Vishnoi, *Advanced Practical Organic Chemistry; Second revised edition*, Vikas Publishing House Pvt. Ltd.
3. A.I. Vogel, *Elementary Practical Organic Chemistry, Part I and II, 2nd edition*, CBS Publication, India
4. R.L. Shriner, R.C. Fuson and D.Y. Curtin, *The Systematic Identification of Organic Compounds; A Laboratory Manual, Fifth edition*, John Wiley and Sons, INC.
5. J. B. Harboren et al, *Phytochemical Methods 2nd edition*, Chapman Hall, London 1984
6. Hostellmann et al, *Preparative Chromatographic Techniques, 2nd edition*, Springer Verlag, Berlin FRG
7. P. J. Houghton and A. Rahman: *A Laboratory Manual for the Fractionation of Natural Extracts*, Chapman Hall, London, 1998

Inorganic Dissertation

Course Title: Inorganic Dissertation
Course No.: Chem 616
Nature of the course: Practical

Full Marks : 50
Pass Marks : 20
The year : II

Course Objective :

- To make the students familiar with research work in inorganic chemistry and related fields.

Course Contents:

Research work on a topic provided by the supervisor

Spectroscopy Electives:

Course Title: Spectroscopy
Course No.: Chem 641
Nature of the course: Theory

Full Marks : 75
Pass Marks : 30
The year : II

Course Objective: To provide advanced knowledge and informations on the applications of different spectroscopic techniques.

Course Contents:

NMR Spectroscopy: The nuclear spin, Larmor frequency, the NMR isotopes, population of nuclear spin levels, spin-spin and spin-lattice relaxation, measurement techniques, solvents used, chemical shift, shielding constants. Use of spin: Spin decoupling technique, use of shift reagents, pulse Fourier Transform technique, proton noise decoupled spectra, off-resonance decoupled spectra, gated decoupling, nuclear Overhauser effect, 2D NMR spectra. Effects of chemical exchange, fluxional molecules, hindered rotation on NMR spectra, Application of ^{19}F , ^{31}P , ^{15}N , ^{11}B , ^{13}C , ^1H spectroscopy to inorganic molecules, temperature effects. **15 hrs.**

Vibration-Rotation Spectroscopy: Microwave spectroscopy of linear polyatomic molecules, Stark effect in microwave spectroscopy, effects of nuclear spins on rotational spectra, selection rules and spectra of symmetric top and asymmetric top molecules. Vibration-rotation spectra: Diatomic molecules: force constants, fundamental vibration frequencies, second and higher harmonics. Vibration-rotation spectroscopy of diatomic molecules, vibration of polyatomic molecules, P, Q, R branches, selection rules, calculation of bond length and effect of isotope substitution in diatomic molecules. Normal modes of vibration, example CO_2 , Absorption of common functional groups. Application to metal ligand vibrations, far IR region, group frequencies of complexed ligands **12 hrs.**

Electronic Spectroscopy : Recapitulation (Beer-Lambert's law, molar extinction coefficient), Oscillator strength and intensity of the electronic transition, the Franck-Condon principle, ground and first excited states of diatomic molecules, fluorescence and phosphorescence, electronic spectra of polyatomic molecules, spectra of transition metal complexes, charge transfer spectra, application of electronic spectroscopy in the characterization of coordination compounds. **10 hrs.**

Electron Spin Resonance Spectroscopy : Theory and instrumentation: Line shapes and line widths of the g-value, origin of hyperfine interaction., Application of ESR in organic, inorganic and organometallic chemistry. **8 hrs.**

Nuclear Quadruple Resonance Spectroscopy (NQR) : Quadruple moments, field gradient, effect of magnetic field on the spectrum, structural information from NQR spectra. **5 hrs.**

Mössbauer Spectroscopy : Introduction, Doppler's effect, instrumentation, chemical application of Mössbauer effects, effect of quadruple moment on the Mössbauer spectrum. **5 hrs.**

Mass Spectroscopy : Instrumentation, ion initiation techniques, identification of molecular ion, isotope ions, factors affecting cleavage patterns, simple cleavage, cleavage at a hetero atom, multicenter fragmentation, McLafferty rearrangements, structure elucidation employing mass spectroscopy, GC-MS, high resolution MS, radical ion mass spectroscopy **8 hrs.**

Symmetry and Group Theory : Symmetry elements and symmetry operations, point groups and molecular symmetry, irreducible representation and character tables, reducible representation, Mulliken's label for representation **15 hrs.**

Uses of Point Group Symmetry in: a. Optical activity, b. Dipole moments, c. Infrared and Raman spectroscopy, and d. Bonding in coordination compounds **2 hrs.**

Reference Books:

1. R.S. Drago, *Physical Methods for Chemists; 2nd Ed.*, Saunders, Fort Worth (1992)
2. E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, *Structural Methods in Inorganic Chemistry*; CRC, Boca Raton Fl (1991).
3. D.C. Harris and M.D. Bertolucci, *Symmetry and Spectroscopy*; Dover, New York (1989).
4. F.A. Cotton, *Chemical Applications of Group Theory: 3rd Ed.*, Wiley, New York (1990),
5. B.E. Douglas and C.A. Hollingsworth, *Symmetry in Bonding and Spectra*; Academic Press, Orlando, FL (1985).
6. K. Nakamoto, *Infrared Spectra of Inorganic and Coordination Compounds*; Wiley, New York.
7. A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions*; Oxford University, New York (1970).
8. H.O. Hill and P. Day, *Physical Methods in Advanced Inorganic Chemistry*; Wiley, New York.
9. C.N. Banwell and E.M. McCash, *Fundamentals of Molecular Spectroscopy: 4th Ed.*, Tata McGraw Hill (1994).

Nuclear Chemistry

Course Title: Nuclear Chemistry
Course No.: Chem 642
Nature of the course: Theory

Full Marks : 75
Pass Marks : 30
The year : II

Course Objective : To provide advanced knowledge on structure and composition of nuclei, radiochemistry, radiation chemistry and important nuclear reactions.

Course Contents:

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. Principal and radial quantum numbers, nuclear parity and nuclear statistics, Nuclear models - the shell model, the liquid-drop model and the collective model.

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, fusion reactors, stellar energy and cold fusion.

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

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

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.

Text Book:

1. H.J. Arnikaar, *Essentials of Nuclear Chemistry 4th Edition*, Wiley - Eastern Limited, 1995.

Reference Books:

1. C. Kellor, *Radiochemistry*; Ellis Norwood Limited, 1988.
2. G.R. Choppin and J. Rydberg, *Nuclear Chemistry, Theory and Applications*; Pergman Press, 1980.
3. An. N. Nesmeyanov, *Radiochemistry*; Mir Publications, 1974.
4. A. K. Srivastava and P.C. Jain, *Elements of Nuclear Chemistry*; S. Chand and Company Ltd. 1983.
5. M. Haissinsky, *Nuclear Chemistry and its applications*; Addison-Wesley Publishing Company, Inc. (1964).
6. G. Friedlander, J.W. Kennedy, E.S. Mahap and J.M. Miller, *Nuclear and Radiochemistry; 3rd edition*, John-Wiley and Sons (1973).
7. E.J. Hall, *Radiation and life*; Pergamon, 1984.

8. B.G. Harvey, *Nuclear Chemistry*; Prentice-Hall, 1965.
9. H.A.C. McKay, *Principles in Radiochemistry*; Butterworths, (1971).
10. K.N. Rao and H.J. Arnikar, *Artificial Radioactivity*; Tata McGraw-Hill (1986).
11. J.W. T. Spinks and R.J. Woods, *An Introduction to Radiation Chemistry*; John Wiley (1976).
12. H. Kiefer and R. Maushart, *Radiation Protection Measurements*; Pergamon Press, (1972).

Natural Product Chemistry

Course Title: Natural Product Chemistry
Course No.: Chem 643
Nature of the course: Theory

Full Marks : 75
Pass Marks : 30
The year : II

Course Objective: To provide broad knowledge on biosynthesis of molecules of nature and on the techniques for their structure elucidation.

Course Contents:

Group A

1. 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
4 hrs.
2. **Phytochemical Techniques:** Extraction, isolation, purification and characterization of natural products
5 hrs.
3. **Primary and Secondary Metabolism:** Introduction, biogenesis of natural products, fatty acid biosynthesis, biosynthesis of polyacetylenes
5 hrs.
4. **Stereochemistry and Biosynthesis:** Chirality and prochirality, chiral methyl groups, hydroxylation at saturated carbon atoms, some reactions of general importance in secondary metabolites, oxidative coupling of phenols, hydroxylation of aromatic substrates, methylation of aromatic substrate
2 hrs.
5. **Biosynthetic Techniques:** Introduction, isotopic labelling by radioactive isotopes and stable isotopes, enzyme and mutant
5 hrs.
6. **Biosynthesis of the following:**
Polyketides: Introduction, formation of poly β -keto acyl CoA's
2 hr.
Terpenes and steroids: Introduction, steroids, pentacyclic triterpenes, squalenes, carotenoids, Vit A
5 hrs.
The shikimic acid pathway: Introduction, quinones, coumarins and flavonoids.
5 hrs.
Alkaloids: Introduction, morphine and related alkaloids
5 hrs.
7. **Microbial metabolites and Antibiotics:** Introduction, piperidine and pyridine metabolite
2 hrs.
8. Bio-assay techniques to screen the natural products, structure-activity relationship
3 hrs.

Group B

9. Classification, extraction, isolation, purification and structure elucidation by chemical and spectroscopic methods and synthesis of the following:
Alkaloids: morphine, colchicine, reserpine
6 hrs.
Terpenes and steroids: phytol, camphor, abietic acid, steroid hormones and contraceptives (progestogen, oestrogen and their derivatives), azadirachtins A and B
6 hrs.
Acetogenin: sciadoptyisin, calistephin chloride, quercetin, baptigenin
6 hrs.

Carbohydrates and glycosides: Preparation of glycoside, chemical properties of glycosides, isolation, degradation, structure elucidation, synthesis of heparin, synthesis of sugars **4 hrs.**

Group C

1. **Isolation, structure elucidation and synthesis of the following:**

Antibiotics: Pencilline, chromycetin, streptomycine and tetracycline

5 hrs.

Vitamin: Vit A, Vit B₁, B₂, B₁₂, Vit C, Vit D and Vit E

6 hrs.

Macromolecules: Natural rubber, resins, natural macrolides (14, 16, 20 and 34 membered macrolides), fatty acids

4 hrs.

Naturally Occurring Organometallic Compounds: Chlorophyll and haemin

4 hrs.

2. **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)

5 hrs.

Reference Books:

1. N.R. Frarlsworth and A.S. Bingel, (Wagner H and Walff P. eds), *New Natural Products and Plant Drugs*; pp 61 –73, springer, New York
2. *Bio activity in Plants: the Link Between Phytochemistry and Medicine*; Phytochemistry, Vol 30, No 12, pp 3864 – 74 (1991)
3. *Methods in Plant Biochemistry*; vol 6, Academic Press, New York
4. I.L. Finar, *Organic Chemistry*; vols. I and II, ELBS Publication
5. W. Herz Ed. *DGI Kingston's Progress in Chemistry of Natural Products*, vol 61, (G. W. Kirby, R. E. Moore etal) Springer Verlag, 1993
6. Atta- Ur- Rahman ed, Synthesis and Structure Activity Relationship of Taxol Derivative as Anticancer Agent; (219, 237, 435, 541 pp), *New trends in Natural Product Chemistry*
7. Nicholas Bodar, *Novel Approaches to Design Safer Drugs*; Academic Press, 256-331pp (1984)
8. W. Hist ed., Coumarins; Murray, Natural Product Report, *Progress in the Chemistry of Organic Natural Products*, Springer Verlag NK (1991)
9. Nakanish, *Natural Product Chemistry*; vols. I, II and III, Academi Press 1975
10. T.A. Geissman, DHG Crout, Freeman, *Organic Chemistry of Secondary Metabolism*; Freeman Cooper and Company, California
11. R.B. Herbert, *Biosynthesis of Secondary Metabolism*; Chapman and Hill Ltd, 1981
12. Leela Dahal, *A Study on Pesticide Pollution in Nepal*; IUCN, NCS Implementaion Project
13. Serge David, *The Molecular and Supramolecular Chemistry of Carbohydrates*, *Chemical Introduction to the Glycosciences*; Oxford University Press (1997)

14. S.W. Pelletier, ed, Chemistry of Alkaloids; (Alumni Foundation Distinguished Professors, Department of Chemistry, The University of Georgia, Athens, Georgia,) Van Nostrand Reinhold Company
15. J.B. Harbone and Helga Mabry Ed, The Flavonoids; Part I and II, Chapman and Hall (1980)
16. 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
17. Human Medicinal Agents from Plants; American Chemical Society, Symposium Series 534, Washington DC, USA 1993
18. Medicinal Plants in Nepal; RDRL Publication, HMG Nepal.

Food Chemistry

Course Title: Food Chemistry
Course No.: Chem 644
Nature of the course: Theory

Full Marks : 75
Pass Marks : 30
The year : II

Course Objective : To provide the students the basic knowledge of food chemistry.

Course Contents:

Group A

1. Recent development in food chemistry. **1 hr.**
2. Moisture in food: chemistry, types, hydrogen bonding, water activity, methods of determination. **5 hrs.**
3. Carbohydrates: definition, classification, monosaccharides (glucose and fructose – structure, general properties. glucose-syrup – manufacture and industrial application) **8 hrs.**
Disaccharides: sucrose, maltose and lactose – structure, properties and uses **5 hrs.**
Polysaccharides: starch - detailed study on its physical, chemical properties and uses. crude fibre (cellulose and hemicellulose) -function and uses. **5 hrs.**
4. Vitamins: classification, chemistry, sources, physiological role (Vit B₂, Niacin, B₆, B₁₂, Biotin, Vitamines D, E, K) with special reference to Vit A; Vit B₁ and Vit C. **6 hrs.**
5. Minerals: occurrence, biochemical function of minerals (Ca, Fe, I₂, Mg, P, Mn, Zn, Na, K) **3 hrs.**

Group B

6. Protein: occurrence, general properties of amino acids, modern concept of protein structure and conformation, denaturation of protein, determination of primary structure, chemical synthesis of peptide and protein., studies of food protein such as milk, meat, wheat and soyabean. **10 hrs.**
7. Enzymes: classification, general properties, coenzymes and cofactors, modern concept of enzymic action, factors affecting enzymic activities, application of enzymes in food industries. **6 hrs.**
8. Lipids: definition, classification, properties of fatty acids and fat, identification of natural fats and oils (melting point, refractive index, iodine value, acid value, saponification value), manufacture of edible oil and vegetable ghee, inter esterification, rancidity – types, mechanism and prevention. **10 hrs.**

Group C

9. Pectic substances: occurrence, structure, pectolytic enzymes, theories of gel formation, uses of pectin. Role of pectolytic enzymes in plant disease. **6 hrs.**

10. Natural pigments: occurrence, chemistry of chlorophyll, carotenoids, anthocyanin, effect of processing and cooking on natural pigments. **6 hrs.**
11. Browning in foods: enzymic browning – mechanism and methods of prevention, non-enzymic browning – types (Maillard caramelization and ascorbic acid browning) – mechanism and methods of prevention. **9 hrs.**
12. Food additives: non-nutritive sweetener (saccharin, thaumatin, aspartame, dihydrochalcone, cyclamate), colouring matter; flavourings (or flavour enhancer eg monosodium glutamate); emulsifiers and stabilizers., antioxidant – Vit E. **10 hrs.**

References

1. Lillian Hoagland Meyer, Food Chemistry; CBS Publishers & Distributors, 1st Indian Edition – 1987.
2. J.B.S. Braverman, Introduction to the Biochemistry of Foods; Elsevier Publication.
3. Lee, Basic Food Chemistry; Avi Publication
4. J.L. Jain Fundamentals of Biochemistry; - 574.192 / J 199f
5. D. Pearson, Laboratory Techniques in Food Analysis; Butterworths
6. G.G. Birch, L.F. Green and C.B. Coulson ed., Glucose Syrups; Applied Science
7. G.G. Birch, L.F. Green and C.B. Coulson ed, Sweetness and Sweeteners; Applied Science
8. O.R. Fennema Food Science Part I, Food Chemistry;
9. N.S. Manay and M. Shadaksharaswamy, Foods - Facts and Principles; New Age International Publishers.
10. N. Pennington and C. W. Baker , Sugar: Users Guide to Sucrose, Chapman and Hall, London. New York, 1990
11. L. W. Aurand and A. E. Woods, Food Chemistry, The AVI publishing Co., Connecticut, 1973.
12. E. A. Davidson, Carbohydrate Chemistry, Holt, New York, 1967.

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