**M.Sc. Chemistry II-Semester CH-502B**

**Inorganic Chemistry –II (Coordination Chemistry)**

| L | T | P | Credits | Sessional Marks: 50 |
|---|---|---|---|---|
| 4 | - | - | 04 | Theory Marks: 100 |
| | | | | Duration of Exams: 3 Hours |

**OBJECTIVES:**

1. To review the basic concepts of electronic states of transition metal complexes.
2. To develop an understanding of calculation of Dq, B and ß parameters
3. To clarify the concept of magnetic properties like magnetic susceptibility and magnetic moments.
4. To understand the effect of an external magnetic field when any transition metal complex comes under its influence.
5. To analyses the stability of a complex compound which is assigned to be existence in aqueous solution w.r.t its bond dissociation energy.
6. To evaluate the rate constant and $E_A$ for substitution reaction.
7. To account parameters for stability of complexes in Thermodynamic and kinetic stabilities.
8. To develop the concept of trans-effect from several theories.
9. To visualize the redox-reaction in octahedral and square planar complexes via outer and inner sphere mechanism.

**OUTCOME:**

- Able to understand the different Spectroscopic ground states in Orgel and Tanabe-Sugano diagrams for transition metal complexes.
- Able to understand the different application of magneto-chemistry in structure determination, magnetic exchange coupling and spin state cross over.
- Able to determine the magnetic susceptibility via Gouy's method. .
- Increased interest in the steps involved in the reaction mechanism of transition metal complexes.
- Able to understand the factors affecting the stability of the metal complexes.

**Books :**


1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huheey, HarperCollins.
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
4. Magnetochemistry, R.L. Carlin, Springer Verlog.
5. Magnetochemistry, A. Earnshaw.
6. Inorganic chemistry, G. Wulf'sburg.
7. Introduction to ligand fields, B.N. Figgis, Wiley Eastern-IIed.
8. Co-ordination Chemsitry, Ajai Kumar
9. General and Inorganic Chemistry, R. Sarkar

**LECTUREWISE PROGRAMME**: **(From 08.01.18 to 27.04.18)**

**M.Sc. Chemistry II-Semester**

**Inorganic Chemistry –II (Coordination Chemistry)Paper No. CH-502 B**

**Credits: 04**

**04 Hrs /week** **External Marks: 100**

**Total: 60 Hrs** **Sessional Marks: 50**

**Duration of Exam: 03 Hrs**

**Note**: The question paper will comprise of eight questions, two from each unit. The candidates will be required to attempt five questions selecting at least one from each unit. All questions will carry equal marks.

**LECTUREWISE PROGRAMME** : (from 08.01.18 to 27.04.18)

**UNIT – I (**from 05.02.18 to 28.02.18)

**Electronic Spectra of Transition Metal Complexes**

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for 1st series of transition metals, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1 – d9 states) calculation of Dq, B and ß parameters, charge transfer spectra of complexes(both metal to ligand and ligand to metal).

**UNIT – II (**from 08.01.18 to 02-02.18)

**Magnetic Properties of transition metal complexes**

Elementary theory of magneto - chemistry, Guoy's method for determination of magnetic susceptibility, calculation of magnetic moments, magnetic properties of free ions, orbital contribution, effect of ligand-field, application of magneto-chemistry in structure determination, magnetic exchange coupling and spin state cross over.

**UNIT – III (**from 01.03.18 to 30.03.18)

**Reaction Mechanism of Transition Metal Complexes - I**

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions.

**UNIT – IV(**from 02.04.18 to 27.04.18)

**Reaction Mechanism of Transition Metal Complexes - II**

Substitution reaction in square planar complexes, the trans effect, mechanism of the substitution reactions. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, inner sphere type reactions**.**

**Metal-Ligand Equilibria in Solution**

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand.

**Home Assignments:** 4 –5 assignments are given during the semester.

**Evaluation Procedure**

| | | |
|---|---|---|
| 1. | Assignment / Performance in the Class | 10 Marks |
| 2. | Minor Tests (Two tests having equal weightage)<br>Minor Test I : 14-16 Feb, 2018<br>Minor Test II : 4 -6 April, 2018 | 40 Marks(20 marks each minor) |
| 3. | University Examination | 100 Marks |

**Award of Grades Based on Absolute Marks:** The University is following the system of grading based on absolute marks (after applying moderation if any). Following grading will be done based on the % of marks obtained in all the components of evaluation part of the subject. A+ (90% - 100 %), A (80% - 89%), B+ (70% - 79%) , B(62% - 69%), C+ (55% - 61%), C (46% - 54%), D (40% - 45), F (Less than 40 %)

For F grade, a candidate shallbe required to appear in the major test of concerned course only in the subsequent examination(s) to obtain the requisite marks/grade.

**Attendance Record –** Candidate should attend at least75% attendance of the total classes held of the subject

**Counselling hour**: 12pm-1pm on Tuesday

**CH-504B Organic Chemistry–II (Structure & Mechanism in Organic Chemistry-2)**

| L | T | P | Credits | Sessional Marks: | 50 |
|---|---|---|---|---|---|
| 4 | - | - | 04 | Theory Marks: | 100 |
| | | | | Duration of Exams: | 3 Hours |

**Teaching Methodology:-** PowerPoint + black board, discussion & solving problems. -

**OBJECTIVES:**

- To introduce students to many of the key concepts of organic chemistry through a survey of the basic reactions of selected monofunctional aliphatic and aromatic molecules.
- To get familiarized with various types of organic reactions.
- To study modern organic chemical reactions and their mechanisms and be able to design synthetic routes to target molecules.
- To review the basic substitution, elimination and addition reaction mechanism as well as fundamental chemistry of carbonyl compounds.

**OUTCOMES:**

- Able to have a firm foundation and application of fundamental concept of organic chemistry.
- Able to recall the fundamental principles of organic chemistry that include chemical bonding, structural isomerism, stereochemistry, chemical reactions and mechanism.
- Expect reaction products and the changes that occur in the structure of organic compounds interacting depending on the type of interaction.
- Understand the influence of bond polarisation on a molecule's structure and reactivity.
- Able to justify a reasonable mechanism for a chemical reaction.

**BOOKS :**


1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundburg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
5. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
6. Advanced Organic Chemistry: Reaction Mechanism, Reinhard Bruckner, Harcourt (India) Pvt. Ltd.
7. Organic reaction Mechanism, V K Ahluwalia and R K Prasher, Narosa Publishing House.
8. Organic Chemistry Vol -1 by Aditi Sangal from Krishna Publishers.
9. Organic reactions and their mechanisms by P S Kalsi New Age International Publishers.
10. Name Reactions Strategic Applications of Named Reactions in Organic Synthesis by Laszlo Kurti (Author), Barbara Czako from Elsevier.
11. Name Reactions and Reagents in Organic Synthesis by Bradford P. Mundy, Michael G. Ellerd and Frank G. Favaloro Jr. from Wiley.
12. Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications by Jie Jack Li from Springer.

13. The Art of Writing Reasonable Organic Reaction Mechanisms by Robert B. Grossman from Springer.

**LECTUREWISE PROGRAMME**: (from 08.01.18 to 27.04.18)

**Introduction of the subject:** **08.01.2018**

**09.01.18- 02.02.18**

**Aliphatic Electrophilic Substitution:**Bimolecular mechanisms – $S_E2$ and $S_Ei$. The $S_E1$ mechanism

**Aliphatic Nucleophilic Substitution:**The $S_N2$, $S_N1$, $S_Ni$, mixed $S_N1$ and $S_N2$ and SET Mechanisms; neighbouring group participation by $\pi$ and $\sigma$ bonds;

**Free Radical Reactions**

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction.

**05.02.18-01.03.18**

**Aliphatic Electrophilic Substitution:** Effect of substrates, leaving group and the solvent polarity on the reactivity.

**Aliphatic Nucleophilic Substitution:** Classical and nonclassical carbocations, phenonium ions, norbornyl system, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium

**Elimination Reactions**: Type of elimination reactions, $E_1$, $E_2$ and $E_{cb}$ Mechanisms.

**Hydrolysis Reactions**: Mechanism of Hydrolysis of esters and amides under acidic and basic conditions.

**05.03.18-30.03.18**

**Aromatic Electrophilic Substitution:** The arenium ion mechanism, orientation and reactivity. The ortho/para ratio, ipso attack, orientation in other ring systems, ambident nucleophile, regioselectivity.

**Aromatic Nucleophilic Substitution:** The $S_NAr$, $S_N1$, benzyne and $S_{RN}1$ mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile.

**Addition to Carbon-Carbon Multiple Bonds:**Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

**02.04.18-27.04.18**

Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

**Addition to Carbon-Hetero Multiple Bonds:** Mechanism of metal hydride reduction of carbonyl compounds, acids and esters. Addition of Grignard reagents, organozinc and

organolithium reagents to carbonyl compounds. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin, Stobbe and Wittig Reaction.

**Evaluation Procedure**

| | | |
|---|---|---|
| 1. | Home assignment | 10 Marks |
| 2. | Minor Tests (Two tests having equal weightage)<br>Minor Test I : 14-16 Feb, 2018<br>Minor Test II : 4 -6 April, 2018 | <br>20 Marks<br>20 Marks |
| 3 | University Examination | 100 Marks |

**Award of Grades Based on Absolute Marks:** The University is following the system of grading based on absolute marks (after applying moderation if any). Following grading will be done based on the % of marks obtained in all the components of evaluation part of the subject.
A+ (90% - 100 %), A (80% - 89%), B+ (70% - 79%) , B(62% - 69%), C+ (55% - 61%), C (46% - 54%), D (40% - 45), F (Less than 40 %)
For F grade, a candidate shall be required to appear in the major test of concerned course only in the subsequent examination(s) to obtain the requisite marks/grade.
**Attendance Record –** Candidate should attend at least75% attendance of the total classes held of the subject
**Chamber consultation hour:** Any vacant period.

**M.Sc. Chemistry II-Semester CH-506B**

**Physical Chemistry -II** (**Kinetics Quantum mechanics and Spectroscopy**)

| L | T | P | Credits | Sessional Marks: 50 |
|---|---|---|---|---|
| 4 | - | - | 04 | Theory Marks:100 |
| | | | | Duration of Exams: 3 Hours |

**OBJECTIVES:**

10. To understand the basic concept of Quantum mechanics with Schrodinger equation.
11. To understand the rate of a reaction and the dependence of rate of reactions on different factors.
12. To develop an understanding of chain reaction.
13. To develop the understanding of different type of catalyst on the chemical reactions and collision theory.
14. To understand the concept of spectroscopy regarding to rotational, vibrational, and electronic.

**OUTCOME:**

- Able to explain the Quantum mechanics operators with Schrodinger equation and their commutation relation.
- Able to explain the rate law of different chemical reactions and affected factors.
- Able to explain the photochemical reaction and general treatment of chain reactions.
- Able to develop the understanding of different types of molecular spectroscopy.

**Books :**


1. Physical Chemistry, P.W. Atkins, Oxford University Press.
2. Physical Chemistry, G.W. Castellan, Narosa. Publishers, New Delhi
3. Principles of Physical Chemistry, Puri, Sharma & Pathania, Vishal Pub.
4. Introductory Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
5. Quantum Chemistry, I.M. Levine, Prentice Hall.
6. Quantum Mechanics, M.L. Strause, Prentice – Hall
7. Quantum Chemistry, J. P. Lowe & K. Peterson, Academic Press (2005).
8. Theoretical Chemistry, Samual Glasstone Affiliated East-West Press.
9. Molecular Quantum Mechanics, P.W. Atkins & R.S. Friedman, 3rd Ed. Oxford University Press (1997).
10. Chemical Kinetics Methods, C. Kalidas, New Age International
11. Chemical Kinetics, K.J. Laidler, McGraw Hill.
12. Modern Spectroscopy, J.M. Hollas, John Wiley.
13. Chemical Applications of Group Theory, F.A. Cotton.
14. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.

15. Basic Principles of Spectroscopy, G.M. Barrow, McGraw Hill.
16. Fundamentals of molecular spectroscopy, C. N. Banwell, Tata Macgraw Hill.
17. Physical Methods in Chemistry, R.S. Drago, Saunders College.

**LECTUREWISE PROGRAMME**: **(From 08.01.18 to 27.04.18)**

**M.Sc. Chemistry II-Semester**

**Physical Chemistry –II** (**Kinetics Quantum mechanics and Spectroscopy**)

**Paper No. CH-506 B** **Credits: 04**
**04 Hrs /week** **External Marks: 100**
**Total: 60 Hrs** **Sessional Marks: 50**
**Duration of Exam: 03 Hrs**

**Note**: The question paper will comprise of eight questions, two from each unit. The candidates will be required to attempt five questions selecting at least one from each unit. All questions will carry equal marks.

**LECTUREWISE PROGRAMME**: (from 08.01.18 to 27.04.18)

**UNIT-I (from 08.01.18 to 02-02.18)**

**Quantum Mechanics**: Postulates of Quantum Mechanics; formulation of Schrodinger wave equation; Max-Born interpretation of and the Heisenberg's uncertainty principle; Quantum mechanical operators and their commutation relation, Hermitian operators, (elementary ideas, quantum mechanical operator for linear momentum and angular momentum as Hermitian operator). The average value of the square of Hermitian operators; commuting operators and uncertainty principle(x & p; E &t); Schrodinger wave equation for a particle in one and three dimensional box; evaluation of average position, average momentum and determination of uncertainty in position and momentum and hence Heisenberg's uncertainty principle, pictorial representation of the wave equation of a particle in one dimensional box and its influence on the kinetic energy of the particle in each successive quantum level, lowest energy of the particle.

**UNIT-II (from 05.02.18 to 28.02.18)**

**Chemical Dynamics I:** Effect of temperature on reaction rates, Rate law for opposing reactions of Ist order and IInd order, Rate law for consecutive Ist order reactions, Collision theory of reaction rates and its limitations, steric factor, Activated complex theory, Ionic reactions: single and double sphere models, influence of solvent and ionic strength, the comparison of collision and activated complex theory.

**UNIT-III (from 01.03.18 to 30.03.18)**

**Chemical Dynamics II:** Chain reactions: hydrogen - bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane. Photochemical reactions (hydrogen - bromine & hydrogen-chlorine reactions). General treatment of chain reactions (ortho -para hydrogen conversion and hydrogen - bromine reactions), apparent activation energy of chain reactions, chain length, Rice-Herzfeld mechanism of organic molecules, decomposition(acetaldehyde) Branching chain reactions and explosions ( H2 - O2 reaction). Kinetics of (one intermediate) enzymatic reaction : Michaelis - Menton treatment, evaluation of Michaelis's constant for

enzyme-substrate binding by Lineweaver - Burk plot, by Dixon and by Eadie-Hofstae methods. Competitive and non-competitive inhibition.

**UNIT-IV (from 02.04.18 to 27.04.18)**

**Spectroscopy:** Electromagnetic radiation, interaction of electromagnetic radiation with matter, regions of the Spectrum, the width and intensity of spectral transitions. Resolving power.

**Rotational spectra:** The rotation molecules, rotational spectra of diatomic molecules, the spectrum of non-rigid rotator, the effect of isotopic substitutions, rotational spectra of linear and symmetric top polyatomic molecules.

**Vibrational and Vibrational – Rotational Spectra:** The vibrating diatomic molecule; simple harmonic vibrations, anharmonicity of vibrations, the diatomic vibrating rotator, the interaction of rotations and vibrations, the vibrations of polyatomic molecules, analysis by infrared technique**.**

**Electronics Spectra:** Electronic spectra of diatomic molecules, vibrational course structure, and rotational fine structure of electronic band, the Frank-Condon principle, intensity of vibrational-electronic band, dissociation energy, organic charge transfer complexes, the Fortrat diagram.

**Home Assignments:** 4 –5 assignments are given during the semester.
**Evaluation Procedure**

| | | |
|---|---|---|
| 1. | Assignment / Performance in the Class | 10 Marks |
| 2. | Minor Tests (Two tests having equal weightage)<br>Minor Test I : 14-16 Feb, 2018<br>Minor Test II : 4 -6 April, 2018 | 40 Marks(20 marks each minor) |
| 3. | University Examination | 100 Marks |

**Award of Grades Based on Absolute Marks:** The University is following the system of grading based on absolute marks (after applying moderation if any). Following grading will be done based on the % of marks obtained in all the components of evaluation part of the subject.
A+ (90% - 100 %), A (80% - 89%), B+ (70% - 79%) , B(62% - 69%), C+ (55% - 61%), C (46% - 54%), D (40% - 45), F (Less than 40 %)

For F grade, a candidate shallbe required to appear in the major test of concerned course only in the subsequent examination(s) to obtain the requisite marks/grade.

**Attendance Record –** Candidate should attend at least75% attendance of the total classes held of the subject

**Counselling hour**: The student can contact in any vacant period.

**M.Sc. Chemistry II-Semester**
**Computer for Chemists**

**Paper No. CH-508 B** **Credits: 03**
**03 Hrs /week** **External Marks: 70**
**Total: 45 Hrs** **Sessional Marks: 30**
**Duration of Exam: 03 Hrs**

**Note**: The question paper will comprise of nine questions, two from each unit. The candidates will be required to attempt five questions selecting at least one from each unit. All questions will carry equal marks.

**LECTUREWISE PROGRAMME** : (from 08.01.18 to 27.04.18)

**UNIT-I(**from 08.01.18 to 28.02.18)

**Computer Fundamentals:** Functional components of a digital computer, concepts of hardware and software, binary, octal & hexadecimal number systems. Binary arithmetic, input/output and storage devices, overview of functions of operating system, types of operating systems, features of windows operating system.

**MS Office:** Word, Excel, Power Point, Equation, Math type.

**Chem Office:** Structure of molecules like proteins, DNA, RNA, Sugar, amino acids, heterocyclic compounds, chemical reactions (single step, two step & multistep) using Chemdraw.

**Programming Fundamentals:** Algorithms, flowcharts, linear and binary search algorithms, bubble sort algorithms. Matrix transpose, matrix addition and matrix multiplication algorithms and their applications.

**UNIT-II (**from 01.03.18 to 27.04.18)

**Programming in C:** Character set, constants and variables, reserved words, data types, expressions, scanf and print statements, operators and their hierarchy, conditional, unconditional and loop control structures. One-dimensional and two-dimensional arrays. Functions.

**UNIT-III (**from 08.01.18 to 28.02.18)

**Computer Application in Chemistry:** Developing programs in C involving simple formulae in chemistry such as van der Waals equation, pH titration, kinetics, radio active decay, evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equation to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge database.

**Books Suggested**


1. Introduction to Computer Science, P.K. Sinha
2. Let Us C, Yashwant Kanetker
3. Computational Chemistry, A.C. Norris.