M.Sc. Chemistry (CBCS) Programme

(Valid from session 2020-21 onwards)

Syllabus

SEMESTER I
M 1 CHE 01-CT01
Inorganic chemistry

Time: 3 Hrs. **M.M. 80 marks (External)**
20 marks (Internal)
Credits = 4

UNIT-I

Stereochemistry and Bonding in Main Group Compounds, VSEPR Theory, Walsh diagrams (tri and penta-atomic molecules), dπ-pπ bonds, Bent rule and enegretics of hybridization, some simple reactions of covalently bonded molecules

Metal-Ligand Bonding: Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory.

UNIT-II

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, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry

UNIT-III

Reaction Mechanism of Transition Metal Complexes: 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 favor of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage.

UNIT-IV

Substitution reactions in square planar complexes, the trans effect, mechanism of the subtitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, inner sphere type reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory.

UNIT-V

Electronic Spectra and Magnetic Properties of Transition Metal Complexes: Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), Calculations of Dq, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Books Recommended:

1. Advanced Inorganic Chemistry, F.A.Cotton and Wilkinson, John Wiley
2. Inorganic Chemistry, J.E.Huhey, Harpes & Row
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, ABP Lever, Elseview
5. Magnetochemistry, R.L. Carlin, Springer Verlag

SEMESTER-I
M 1 CHE 02-CT02
Organic Chemistry

Time: 3 Hrs. **M.M. 80 marks (External)**
20 marks (Internal)
Credits 4

UNIT-I

Nature of bonding in organic molecules: Delocalized chemical bonding-conjugation, cross conjugation, bonding in fullerenes, aromaticity in benzenoid and non-benzenoid compounds, annulenes, ferrocenes and helicenes, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of Π-molecular orbitals, anti-aromaticity, Homo-aromaticity.

UNIT-II

Reaction mechanism, structure and reactivity - A review of types of mechanisms and reaction, Methods of determining mechanisms, Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, Generation, Structure, Stability and reactivity of reactive intermediates, isotope effects, effect of structure on reactivity-resonance and field effects, steric effect, steric inhibition to resonance, substituent and reaction constants, Hammett and Taft equation.

UNIT-III

Aliphatic reaction Mechanism

(i) Nucleophilic substitution - The S_N2, S_N1, mixed S_N2 and S_N1, S_Ni and SET mechanisms, Neighbouring group participation.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation, rearrangements, nucleophilic substitution at allylic, trigonal and vinylic carbon, reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambient nucleophile, regioselectivity.

(ii) Electrophilic substitution – S_E2 and S_E1 mechanism, electrophilic substitution accompanied by double bond shift, effect of substrates, leaving group and the solvent polarity on reactivity.

UNIT-IV

Aromatic reaction Mechanism

(i) Electrophilic substitution - The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, diazonium coupling, Vilsmeir - Haak reaction, Bischler-Napieralski reaction, Pechmann reaction.

(ii) Nucleophilic substitution - The S_NAr, S_N1, benzyne and SR_N1 mechanisms, reactivity - effect of substrate structure, leaving group and attacking nucleophile. Von Richter, Sommelet-Hauser and Smiles rearrangements.

(iii) Free radical reaction - Types of free radical reactions, free radical substitution mechanism, neighboring group assistance, reactivity for aliphatic and aromatic substrate at a bridgehead, reactivity in the attacking radicals, the effect of solvents on reactivity, allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

UNIT-V

Addition Reaction

Carbon-Carbon multiple bonds - Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity, addition to cyclopropane ring, hydrogenation of double bond, triple bonds and aromatic rings, hydroboration, Michael reaction.

Carbon-Hetero multiple bonds - Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, mechansim of condensation reaction involving enolates- Aldol, knoevengel, Mannich, Benzoin, Perkin and Stobbe reactions.

Elimination reaction - The E2, E1, ElcB and E2cB mechanisms, orientation of the double bond, reactivity-effect of substrate structures, attacking base, the leaving group and the medium, stereochemistry, elimination v/s substitutions, pyrolytic eliminations.

Books Recommended :

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum
3. A Guide book of Mechanism in Organic Chemistry, Peter Sykes, Longman
4. Structure and Mechanism in Organic Chemistry, Peter Sykes, Longman
5. Modern Organic Reactions, H.O. House, Benjamin
6. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional
7. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh Macmillan.
8. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
9. Stereochemistry of Organic Compounds, P.S Kalsi, New age International
10. Organic Reaction and Their Mechanisms, P.S. Kalsi, New Age International
11. Organic Reaction Mechanism, V.K. Ahluwalia and R.K. Parshar, New Age International.

SEMESTER-I
M 1 CHE 03-CT 03
Physical Chemistry

Time: 3 Hrs. **M.M. 80 marks (External)**
20 marks (Internal)
Credits 4

ESSENTIAL –All students must have knowledge of these topics of mathematics-

Differentiation and Integration of some simple terms, Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigenvalue problem, orthonormal sets, Fourier and Laplace transforms.

UNIT-I

Quantum chemistry: The Schrodinger equation and the postulates of quantum mechanics, solutions of the Schrodinger equation to some model system viz. particle in a box, the harmonic oscillator.

Approximate methods: First order time-independent perturbation theory for non- degenerate states. Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

UNIT-II

Angular momentum: Ordinary angular momentum, generalized angular momentum, eigen functions and eigen values of angular momentum, operators, algebra of operators, ladder operators, addition of angular momenta, spin, antisymmetry and Pauli's exclusion principle.

Electronic structure of atoms: Electronic configuration, Russell-Saunder's terms and coupling schemes, molecular orbital theory, Huckel theory of conjugated systems, bond order and charge density calculations, application to ethylene, allyl and cyclobutadiene systems.

UNIT-III

Chemical dynamics: Methods of determining rate laws and mechanism, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and thermodynamic parameters, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, dynamics of unimolecular reactions.

UNIT IV

Catalysis, homogeneous and heterogeneous catalysis, kinetics of enzyme reactions, chain reactions, photochemical chain reactions (Hydrogen-bromine and hydrogen-chlorine reactions) oscillatory reactions (Belousov-Zhabotinsky reaction), general features of fast reactions.

UNIT V

Macromolecules: Definition, types of polymers, electrically conducting, fire resistant and liquid crystal polymers, kinetics of polymerization, mechanism of polymerization, molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods, GPC), sedimentation.

Books Recommended:

1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).

2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt. Ltd.: New Delhi (2003).

3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).

4. Pilar, F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).

5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press

6. Levine, I. L Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).

7. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).

8. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).

9. Chemical Kinetics, K.J. Laidler, Mcgraw-Hill.

10. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.

SEMESTER-I
M 1 CHE 04-CT 04
Group Theory and Spectroscopy

Time: 3 Hrs. **M.M. 80 marks (External)**
20 marks (Internal)
Credits 4

UNIT I

Symmetry and Group theory in Chemistry:

Symmetry elements and symmetry operation, definition of group, subgroup, Conjugacy relation and classes. Point symmetry group, Schonfilies symbols, representation of groups by matrices (representation for the $C_{\eta h}$, $C_{\eta v,}$ etc. groups to be worked out explicitly). Characters of a representations, Great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy, Derivation of character table for C_{2v} and C_{3v} point group, symmetry aspects of molecular vibrations of H_2O molecule.

UNIT-II

Unifying Principles: Electromagnetic radiations, Interaction of electromagnetic radiation with matter, Uncertanity relation and natural line width, Factors affecting natural line width. **Rotational spectroscopy:** Classification of molecules, rigid rotator, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, stark effect, nuclear and electron spin interaction and effect of external field, applications.

UNIT III

Vibrational Spectroscopy:

Infra red spectroscopy

Review of linear harmonic oscillator, Vibrational energies of diatomic molecules, Zero Point energy, force constant and bond strength, anharmonicity, Morse Potential energy diagram, Vibration-rotation spectroscopy, P.Q.R. branches, breakdown of oppenheimer approximation, selection rules, finger print region, Group frequencies and intensities, overtones, hot bands, combination bands and Fermi resonance.

Raman spectroscopy: Classical and quantum theories of Raman effect, Stokes and anti-Stokes lines, Pure rotational, vibrational, rotational- vibrational Raman spectra, Mutual exclusion principle.

UNIT IV

Electronic spectroscopy

Atomic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Molecular Spectroscopy

Electronic spectra of diatomic molecules: Born oppenheimer approximation, vibrational progressions, Franck-Condon principle. Electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Photoelectron Spectroscopy: Basic principles, photo-electric effect, ionization process, Koopman's theorem, ESCA-theory, Auger emission spectroscopy –Basic idea.

Unit V

Mössbauer Spectroscopy: Basic principles, Instrumentation, Lamb-Mossbauer factor, Mossbauer nuclides, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds - nature of M-L bond, -coordination number, structure (3) detection of oxidation state and equivalent MB atoms.

Books recommended-

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Chemical Applications of Group Theory, F. A. Cotton.
3. Symmetry and Group theory: Some chemical applications, Ramashankar and Suresh Ameta, Himanshu Publications, Udaipur, Delhi.
4. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.

6. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH- Oxford.
7. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
8. Introduction to Magnetic Resonance, A Carrington and A.D. Maclachalan, Harper & Row.
9. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
10. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.

SEMESTER-I

M1 CHE 05-CP 01 (Core practical I) Credits 4; Time 8h

M.M. 80 marks (External)
20 marks (Internal)

1. **Separation of binary mixture (minimum -8) (30 Marks)**
   Purification and identification of compounds in a binary mixture of two solids or solid-liquid and preparation of their suitable derivatives
2. **One Step Organic Synthesis (minimum -4) (10 Marks)**

(One experiment to be performed from the following in the examination)

I. Acetylation- Acetylation of Salicylic acid using acetyl chloride

II. Benzoylation- Benzoylation of phenol/ aniline/ glycine

III. Oxidation- Phenanthroquinone from Phenanthrene

IV. Sandmayer Reaction- o-Chlorotoluene from o-Toluidine

V. Acetoacetic ester Condensation- Synthesis of ethyl-n-butylacetoacetate

VI. Bromination Reaction- to prepare dibromoflurorescein from fluorescein.

VII. Claisen-Schmidt Condensation- Benzalacetophenone/Bezalacetone/ diBenzalacetone from Benzaldehyde

3. **Two step Organic Synthesis (minimum -2) (20 Marks)**

I . Preapration of Acetanilide from Acetophenone (Beckmann Rearrangement)

II. Preapration of *m*-Nitroaniline from nitrobenzene

III. Preapration of *m*-phenylenediamine from nitrobenzene

IV. Preapration of Methyl orange from aniline

4. Viva (10 Marks)

5. Record (10 Marks)

SEMESTER-I

M 1 CHE 06-CP 02 (Core Practical-2) **Credits 4; Time 8 h**

M.M. 80 marks (External)

20 marks (Internal)

1. Qualitative analysis of Inorganic mixture– (minimum -6)

Qualitative analysis of inorganic mixture containing SIX radicals from the following list: (at least three from Group B)

Group A - Carbonate, Sulphite, Sulphate, Sulphide, Nitrite, Acetate, Oxalate, Nitrate, Chloride, Iodide, Phosphate, Fluoride, Borate, Silver, Lead Mercury, Bismuth, Copper, Cadmium, Tin, Arsenic, Antimony, Aluminium, Chromium, Iron, Nickel, Cobalt, Zinc, Manganese, Calcium, Barium, Strontium, Magnesium, Ammonium.

Group B - Thiosulphate, Cyanate, Thiocyanate, Hypochlorite, Chlorate, Percholrate, Iodate, Persulphate, Silicate, Chromate, Arsenate, Benzoate, Thalium, Tungsten, Molybdenum, Vanadium, Beryllium, Uranium, Thorium, Titanium, Zirconium, Cerium.

1. Kinetics – (minimum -4)

I. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate by the Initial Rate Method.

II. Compare the strengths of hydrochloric acid and sulphuric acid by studying rate of hydrolysis of methyl acetate.

III. Determine the specific reaction rate constant of the potassium persulphate-iodide reaction by the Initial Rate Methods.

IV. Study the kinetics of the iodination of acetone in the presence of acid by the Initial rate Method.

2. Conductometry – (minimum -4)

I. Determine the equivalent conductance, degree of dissociation, dissociation constant (K_a) for weak electrolytes (CH_3COOH, NH_4OH) and verify Ostwald dilution law.

II. Determine the solubility of sparingly soluble salt and its solubility product.

III. Study the conductometric titration of hydrochloric acid with sodium carbonate and determine the concentration of sodium carbonate in a commercial sample of soda ash.

IV. Determine basicity of weak organic acid.

V. Determine the strength of strong and weak acids in a given mixture.