# OUTLINES FOR MS/ MPHIL SUBJECT TEST DEPARTMENT OF CHEMISTRY UNIVERSITY OF OKARA

Following are the outlines from which MS/MPhil subject will be formulated. The pattern for the test will be MCQ's type.

# **Organic Chemistry**

### **Basic Concepts of Organic Chemistry:**

Bonding and hybridization, localized and delocalized bonding, structure-aromaticity, inductive effect, dipole moment, resonance and its rules, hyperconjugation, classification and nomenclature of organic compounds including IUPAC system, types of organic reactions (an overview).

#### **Chemistry of Hydrocarbons:**

Saturated, unsaturated and aromatic hydrocarbons with emphasis on synthesis and free radical, electrophilic addition and electrophilic substitution reactions.

### **Chemistry of Functional Groups:**

Hydroxyl, ether and amino groups, preparation and properties of alcohols, phenols, ethers, and amines with focus on reaction mechanism and applications, carbonyl compounds, preparations and reaction mechanism of aldehydes and ketones and their applications, carboxylic acids and their derivatives, acidity of carboxylic acids and effect of substituents on their acidity, preparation and reactions of carboxylic acids and their derivatives including esters, amides, acid halides and acid anhydrides.

#### **Stereochemistry:**

Types of stereoisomers, DL Conventions, RS, Cis-Trans, EZ notation Syn-Anti configuration, optical activity, stereoselectivity and stereospecificity, Felcon Ahn model, chiral compounds having no chiral centre e.g. spiro compounds and biphenyls, conformational analysis of ethan, propane, butane, cyclohexane, mono and di substituted cyclohexane, decaline.

#### **Organic Reactions and Mechanism:**

Detailed mechanism of aliphatic reactions including addition, substitution, and elimination reactions, concept of energy profile, transition state and intermediate.

#### **Aromatic Substitution Reactions:**

Mechanisms of aromatic reactions including electrophilic like nitration, sulphonation, halogenation, alkylation, acylation, formylation, caboxylation and nucleophilic substitutions, effect of substituents on orientation and reactivity.

#### **Oxidation-reductions Reactions:**

Common oxidizing and reducing reagents, reactions involving elimination of H, cleavage of C-C bond, replacement of hydrogen by oxygen, and addition of oxygen to substrates, reaction involving replacement of oxygen by hydrogen, removal of oxygen from the substrates and reduction with cleavage.

#### **Pericyclic Reactions:**

Introduction to pericyclic reactions, frontier orbital theory, mechanisms of electrocyclic, cycloaddition and sigmatropic reactions.

# **Physical Chemistry**

## **Chemical Thermodynamics:**

Equation of states, ideal and real gases, the virial equation and the van der Waals equation for real gases, critical phenomena and critical constants, four laws of thermodynamics and their applications, thermochemistry, calorimetry, heat capacities and their dependence on temperature, pressure and volume, reversible and non-reversible processes, spontaneous and non-spontaneous processes, relations of entropy and Gibbs free energy with equilibrium constant, Gibbs Helmholtz equation.

#### **Chemical Equilibrium:**

General equilibrium expressions, reaction quotients, examples of equilibrium reactions in solid, liquid and gas phases, extent of reactions and equilibrium constants, Gibbs energies of formation and calculations of equilibrium constants, Le-Chatelier's principle, effect of temperature, pressure and compositions on the equilibrium constants, van't Hoff equation,.

### **Solution Chemistry:**

Physical properties of liquids, surface tension, viscosity, refractive index, dipole moment etc. and their applications, brief account of interactions among the molecules in liquids, ideal and non-ideal solutions, Raoult's law and its applications, lowering of vapor pressure, elevation of boiling point, depression of freezing point, osmotic pressure and its measurement, vapor pressure of non-ideal solutions and Henry's law, abnormal colligative properties, fractional distillation and concept of azeotropic mixtures.

#### **Chemical Kinetics:**

The rates of reactions, zero, first, second and third order reactions with same and different initial concentrations, half-lives of reactions, experimental techniques for rate determination and methods for determination of order of reaction Arrhenius equation.

#### **Quantum Chemistry:**

Black body radiation, photoelectric effect, line spectra of elements, Bohr atomic model, wave and particle nature of matter, de Broglie's equation, Young's double slit experiment, Heisenberg's uncertainty principle, wavefunctions and Born interpretation of wavefunctions, probability density, eigen functions and eigen values, Schrödinger wave equation, Hamiltonian operator, wavefunctions for hydrogen-like atomic orbitals, radial distribution functions, shielding and penetration, effective nuclear charge, orbital energies.

### **Kinetic Theory of Gases:**

Probability density for molecular speeds of gas molecules, Maxwell distribution of molecular speeds, average speeds, pressure of an ideal gas, calculation of molecular speeds, binary collisions, effusion and mean free paths, Maxwell-Boltzmann's law of energy distribution, method for the determination of the Avogadro's number (NA), statistical probability and entropy.

#### **Phase Equilibrium:**

Gibbs phase rule, Phase diagrams of one component and two component systems, Gibbs energy and the phase diagram of a substance, location of phase boundaries, Clausius-Clapeyron equation, vapor-liquid equilibrium of binary liquid mixtures, binary phase diagrams and lever rule.

### **Conductometry:**

Ions in solution, measurement of conductance and Kohlrausch's law, mobility of ions and transport number, conductometric titrations, Debye-Hückel theory and activity coefficient, determination of activities, application of conductance measurement.

### **Electrochemistry:**

Redox reactions, spontaneous reactions, electrochemical cells, standard electrode potentials, liquid junction potential, electrochemical series, Nernst's equation, thermodynamic of redox reactions, Latimer Diagram, Frost Diagram, electrolytic cells, potentiometry, reference and indicator electrodes, corrosion and its prevention, fuel cell and hydrogen economy.

### **Surface Chemistry:**

Interfaces, Gibbs surface excess, curved surfaces, capillary action, adsorption and adsorption isotherms, Freundlich and Langmuir adsorption isotherms, catalysis, colloids, emulsion and their industrial applications.

### **Nuclear Chemistry:**

Atomic nucleus, nuclear stability, modes of decay, nuclear energetics, nuclear models (shell + liquid drop model), fusion and fission, non- spontaneous nuclear processes, nuclear reactors.

# **Inorganic Chemistry**

# **Periodicity:**

Modern periodic table; Similarities and differences in first row elements, their diagonal and vertical relationship with other elements; Electro negativity of elements (Pauling and Mullikan scales); Polarizability and polarizing power of ions; Periodicity in the properties of transition and inner transition elements.

#### **Chemical Bonding:**

Types of chemical bonding, ionic and covalent bonding, localized bond approach, theories of chemical bonding, valence bond theory (VBT), hybridization and resonance, prediction of molecular shapes using Valence Shell Electron Pair Repulsion (VSEPR) model, molecular orbital theory (MOT) applied to diatomic molecules, delocalized approach to bonding, bonding in electron deficient compounds, hydrogen bonding.

#### **Acids and Bases:**

Brief concepts of chemical equilibrium, acids and bases including soft and hard acids and bases (SHAB), concept of relative strength of acids and bases, significance of pH, pKa, pKb and buffer solutions, theory of indicators.

#### **p-Block Elements**:

Physical and chemical properties of p-block elements with emphasis on some representative compounds.

### Chemistry of d-block elements and coordination complexes:

Back ground of coordination chemistry, nomenclature and structure of coordination complexes with coordination number 2-6, chelates and chelate effect, theories of coordination complexes, Werner's theory, valence bond theory (VBT), crystal field theory (CFT) and molecular orbital theory (MOT), Jahn-Teller theorem, magnetic properties, spectral properties, isomerism, stereochemistry, and stability constants of coordination complexes.

#### **Chemistry of f-block elements:**

(i) Lanthanides: General characteristics, occurrence, extraction and general principles of separation, electronic structure and position in the periodic table, lanthanides contraction, oxidation states, spectral and magnetic properties and uses. (ii) Actinides: General characteristics, electronic structure, oxidation state and position in the periodic table, half-life and decay law.

### **Inorganic materials:**

Crystalline and amorphous states, design of inorganic materials and characterization, X-ray spectra and N(E) curves, n(E) curves. Metallic bond on the basis of band model, Binding energy in metals, conductors, semi-conductors and insulators. Effect of temperature and impurities on conductivity. Doping and purification of silicone, chemical vapour deposition and sputtering, introduction to nano materials.

# Pi- acceptor Ligands:

Transition metal carbonyls (Mononuclear, Binuclear, Poylnuclear), synthesis, bonding situation based on spectroscopic evidences; Theoretical rationalization of molecular structures, (close, nido, erachno), Synthesis. Characteristics and reactivity of derivatives of metal carbonyls (carbonylate anions, carbonyl hydrides and carbonyl halides); Metal nitrosyls including halonitrosyl and their derivatives.

# **Analytical Chemistry**

#### Chemeomtrics

Introduction and scope of Analytical Chemistry: Analytical problems and their solutions; The nature of analytical methods; trends in analytical methods; Different units of concentration and their conversion; Definition and basic concepts: nature and origin of errors, Classification of errors; Accuracy and Precision; Limits of detection, Confidence limits; Deviation, Standard deviation, Application of statistical tests; Rounding off analytical data; Computation of analytical data. Significance of sampling, weighing and measuring in Analytical chemistry.

#### **Classical Analytical Methods:**

Acid-base, complexometric and redox titrations, gravimetric analysis.

#### **Modern Analytical Methods:**

Classifications of Chromatographic Techniques, Paper and Thin Layer Chromatographic Techniques; their instrumentation, applications and limitations, Column Adsorption Chromatography, Introduction to Molecular spectroscopy, absorption in UV and Visible range; Basic principle of Spectrophotometry; Beer-Lambert's law; Deviations; Instrumentation and application.

#### **Separation Methods:**

Cation Exchange resin, Anion Exchange resin, Cross-linkage, Separation of metal ions on Anions Exchange Columns, Applications of ion Exchange Chromatography. Basic principle of solvent extraction, The Distribution Coefficient, The Distribution Ratio, Solid-Phase Extraction, Solvent Extraction by Flow Injection Analysis. Capillary Zone Electrophoresis, Application of traditional Electrophoresis, Gel Chromatography.

#### **Analytical Spectrophotometry:**

Properties of light and its interaction with matter, relation between frequency, velocity and wave number, Lambert- Beer's law and its limitations, single beam and double beam spectrophotometers, lamps and lasers as sources of light, monochromators, detectors, photomultiplier tube, photodiode array, charged coupled device, FT-IR spectroscopy, Fourier analysis, interferometry, noise and its control.

# **Applied Chemistry**

### **Fundamentals of Chemical Industry:**

Basic principles and parameters for industrial plant unit operations and unit processes.

#### **Chemical Industries:**

Raw materials, flow sheet diagrams and unit operations and unit processes of sulphuric acid, nitric acid, hydrochloric acid, oxalic acid, formic acid, caustic soda and washing soda, cement industry, petroleum, textile, polymer and fuel industries, applications of these industries.