K.V.R GOVERNMENT COLLEGE FOR WOMEN (A), KURNOOL
M Sc. ORGANIC CHEMISTRY
I SEMESTER SYLLABUS under CBCS
EFFECTIVE FROM THE ACADEMIC YEAR 2021-2022
CHEM- 101: PAPER-I INORGANIC CHEMISTRY –I

UNIT-I: COORDINATION COMPOUNDS

Coordination compounds: crystal field splitting patterns in tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series, Jahn - Teller effect,limitations. Nephelauxetic effect – ligand field theory.Term symbols – Russell – Sanders coupling, derivation of term symbols for various configurations. Spectroscopic ground states.

UNIT-II: INORGANIC CAGE AND RING COMPOUNDS

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallo carboranes, boron–nitrogen ($H_3B_3N_3H_3$), phosphorus–nitrogen ($N_3P_3Cl_6$) and cyclic sulphur-nitrogen (S_4N_4, $(SN)_x$) compounds.Electron counting in boranes – Wades rules (Polyhedral skeletal electron pair theory).Isopoly and heteropoly acids (elementrary treatment)

UNIT-III: STRUCTURE & BONDING

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in pi bonding.

Application of MO theory to square planar ($PtCl_4^{2-}$) and Octahedral complexes (CoF_6^{3-}, $Co(NH_3)_6^{3+}$).

UNIT- IV: ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES

Electronic spectra of transition metal complexes: Selection rules, breakdown of selection rules – Orgel and Tanabe-Sugano diagrams for d^1 –d^9 octahedral and tetrahedral transition metal complexes of 3d series – Calculation of Dq, B and β parameters. Charge transfer spectra.

Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes.

Books Suggested:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)

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CHEM-102: PAPER-II ORGANIC CHEMISTRY –I

UNIT-I: STEREO CHEMISTRY

Concept of Chirality: Recognition of symmetry elements and chiral structures (one and more than one chiral centers); D,L and R,S nomenclature, diastereoisomerism; Inter-conversion of Fischer, Newman and Sawhorse projections. Threo and Erythro isomers, Optical activity in the absence of chiral carbon axial chirality (allenes and spiranes).Atrope isomerism(biphenyls) helicity, Recemic Modifications –- methods of resolution - Nature and formation of recemic modifications – by mixing, by synthesis, by recemization, by chemical tranformations Geometrical isomerism-E, Z nomenclature. physical and chemical methods of determining the configuration of geometrical isomers.

UNIT-II: NATURE OF BONDING & AROMATICITY

NATURE OF BONDING

Delocalised chemical bonding conjugation,acidity and basicity of organic molecules, cross conjugation, hyper conjugation, Tautomerism, mesomeric effect

Aromaticity: Concept of Aromaticity, Aromaticity of five membered, six membered rings and fused systems.-Non benzonoid aromatic compounds:-cyclopropenylcation, Cyclobutadienyldication, cyclopentadienyl anion-tropylliumcation and cyclooctatetraenyldianion, Metallocenes, Ferrocene, Azulenes, Fulvenes, Annulenes, Fullerenes, Homoaromaticity, Antiaromaticity and pseudo aromaticity.

Unit –III: REACTIVE INTERMEDIATES

Generation, Structure, Stability,Detection and Reactivity of Carbocations, Carbanions, Free radicals, Carbenes, Nitrenes and Arynes. Reactive Species: Generation and reactivity of Electrophiles, Nucleophiles, Dienophiles, Ylids,Enophiles.

UNIT-IV: REACTION MECHANISM-I

(a) **Addition reactions:** Introduction, addition reactions involving electrophiles (Br_2, HBr, HOBr & H_2O/H_2SO_4), Addition reactions involving Nucleophiles, Free radical additions-Kharash peroxide effect. Stereo specificity in addition reactions: Bromination,Dihydroxylation, Hydroboration, hydrogenation reactions Syn-addition of OsO_4& KMnO4

(b) Introduction of Nucleophilic substitution reactions:

SN^1, SN^2&SN^i-Mechanisms & stereochemistry-factors affecting the rate of SN^1& SN^2 reactions such as substrate structure, nature of leaving group, nucleophile & the solvent, neighbouring group participation.

Books Suggested:

1. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International).
2. Aromatic Character & aromaticity, G.M.Badger
3. Organic reaction mechanism, V.K.Ahluwalia, R.K.Parashar.
4. Organic reactions with mechanisms, S.P.Bhutani

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CHEM- 103: PAPER-III PHYSICAL CHEMISTRY –I

UNIT-I: THERMODYNAMICS-I

Chemical equilibrium- effect of temperature on equilibrium constant-Van't Hoff equation. Partial molar quantity- different methods of determination of partial molar quantity. Chemical potential- Phase rule and its derivation, Gibbs-Duhem equation, Duhem-Margules equation, Classius-Clapeyron equation. Nernst heat theorem. Third law of thermodynamics- Determination of the absolute entropy- Apparent exceptions to Third law of thermodynamics.

Unit-II: polymers

Thermodynamics of polymer dissolution, effect of molecular weights on solubility, solubility of crystalline and amorphous polymers, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins Theory of polymers solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular mass-Number and mass average molecular mass, molecular weight determination by ultracentrifugation, sedimentation equilibrium method.

UNIT -III: CHEMICAL KINETICS-I

Theories of reaction rates: Collision theory, steric factor. Theory of Absolute Reaction Rates-Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reacton rates.

Unimolecular reactions: Lindemann, Lindemann-Hinshel wood, and RRKM theories. Termolecular reactions. Complex reactions-Rate expressions for opposing, parallel and consecutive reaction (all first order type)

Chain reactions: Dynamic chain, hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane, photochemical reactions- H_2-Br_2, H_2-Cl_2 reactions, Autocatalysis, H_2-O_2 reaction explosion limits.

Fast Reactions: Flow system – Temperature and pressure Jump Methods – Relaxation Techniques.

UNIT – IV: ELECTROCHEMISTRY-I

Reversible cells – Chemical cells and concentration cells – Types of reversible electrodes – Electrode potentials. Reactions in reversible cells – Nernst equation – thermodynamic and kinetic derivation – Concentration cells with and without transference.

Liquid junction potential and its determination.Potentiometric titrations – Determination of pH, Solubility product from EMF measurements.

Theory of electrolytic conductance – Debye - Huckel Onsager equation and its verification – Wein effect. Conductometric titrations, Determination of solubility of a sparingly soluble salt.

Books Suggested:

1. A text Book of Physical Chemistry (2nd Ed.), S. Glasstone (Macmilan)
2. Polymer Chemistry, Gowarikar.
3. Chemical Kinetics, K.J. Laidler.
4. Atkin's Physical Chemistry, Peter Atkins and Julio de paula.

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CHEM- 104: PAPER-IV GENERAL CHEMISTRY-I

UNIT-I: GROUP THEORY

Symmetry elements and symmetry operations; Point groups; Mathematical requirements for a point group; Schoenflies notation of point groups; assignment of point groups; Group Multiplication table of C_{2V}, C_{3V} and C_{2h} point groups; Reducible and Irreducible representations, Mullikan notation for Irreducible representations, Great orthogonality theorem (without proof), Character tables, Application of character tables for C_{2V} and $C_{3V}$for prediction of stereochemistry of cis-trans C_{2h} molecules.

UNIT-II: MICROWAVE SPECTROSCOPY

Diatomic molecules- rigid rotator, Selection rules. Intensity of spectral lines. Effect of isotopic substitution-calculation of bond length, intensities, non-rigid rotator, polyatomic molecules- Classification of molecules -Spectra of linear and symmetric top molecules. Stark Effect.

UNIT-III: INFRARED SPECTROSCOPY & RAMAN SPECTROSCOPY

Infrared spectroscopy: Harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combination bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.Vibrations of simple, poly atomic molecules CO2, H2O.

Raman spectroscopy: Classical and quantum theories of Raman Effect, pure rotational, pure vibrational Raman spectra, selection rules, mutual exclusion principle. Vibrational - rotational Raman spectroscopy.

UNIT-IV: ELECTRONIC SPECTROSCOPY

Line spectra and band spectra, selection rules for electronic transition, Coarse structure, Band head and shading formation, Fine Spectra, Effect of vibrational spectra on electronic spectra, effect of vibrational-rotational spectra on electronic spectra of homo nuclear and hetero nuclear diatomic molecules.

Books Suggested:

1. Introduction to Quantum Chemistry, A.K.Chandra (Tata Mc Graw Hill).
2. Quantum Chemistry, Iran. Levine (Prentice Hall).
3. Fundamentals of Molecular Spectroscopy-C.N.Banwell (Mc Graw Hill).
4. Molecular structure and Spectroscopy-G.Aruldhas.
5. Atomic structure and chemical bond including molecular spectroscopy-Manas Chanda.

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CHEM- 201: PAPER-I INORGANIC CHEMISTRY –II

UNIT-I: METAL CLUSTER COMPOUNDS

Definition – evidences for existence of M-M bonds - conditions favorable for formation of M-M bonds – preparation, structure and bonding of the following metal cluster compounds.

$Re_2Cl_8^{2-}$, $Mo_2Cl_8^{4-}$, $Re_2(RCOO)_4X_2$, $Mo_2(RCOO)_4(H_2O)_2$, $Cr_2(RCOO)_4(H_2O)_2$, $Cu_2(RCOO)_4$ $(H_2O)_2$, $Cr_2Cl_9^{3-}$, $Mo_2Cl_9^{3-}$, $W_2Cl_9^{3-}$, Re_3Cl_9, $Re_3Cl_{12}^{3-}$, $Mo_6Cl_8^{4+}$, $Nb_6X_{12}^{2+}$ and $Ta_6X_{12}^{2+}$.

UNIT-II: ORGANOMETALLIC COMPOUNDS - 16 and 18 electron rules.

Isoelectronic relationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen and nitric oxide complexes.

Isolobal relationship – H, Cl, CH_3, $Mn(CO)_5$; S, CH_2, $Fe(CO)_4$; P, CH, $Co(CO)_3$

Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene.

UNIT-III: METAL LIGAND EQUILIBRIA IN SOLUTION

Step wise and overall formation constants and their interaction – trends in stepwise constants – factors affecting the stability of metal complexes – Pearson's theory of hard and soft acids and bases (HSAB), chelate effect and its thermodynamic origin, determination of stability constants of complexes – spectrophotometric method and pH –metric method.

UNIT- IV: INORGANIC REACTION MECHANISM

Reactivity of metal complexes – inert and labile complexes. Explanation of lability on the basis of valence bond and crystal field theories.

Substitution reactions of metal complexes – D, Id, Ia and A mechanisms – Ligand replacement reactions of metal complexes – Acid hydrolysis – factors affecting acid hydrolysis – Anation and Base hydrolysis of Cobalt(III) complexes. Ligand displacement reactions of square planar complexes of platinum (II). Factors affecting square planar substitution – trans effect (theories).Electron transfer reactions of complexes – concept of complementary and non-complementary reactions with examples. Inner and outer sphere mechanisms.

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CHEM-202: PAPER-II ORGANIC CHEMISTRY- II

UNIT-1 MOLECULAR REARRNGMENENTS

Introduction, types of molecular rearrangements.

1. Rearrangements to electron deficient carbon atom: Pinacol-pinacolone , Demjonove, Wagner-Meerwein
2. Rearrangement to electron deficient nitrogen atom
   Beckmann, Hoffmann, Curtius, Claisen-Schmidt& Lossen rearrangement
3. Rearrangements to electron deficient oxygen atom
   Baeyer-villiger and Dakins rearrangements
4. Rearrangements to electron rich atom
   Favorski and Neber rearrangements

UNIT-II ELIMINATION REACTIONS

E1, E2, E1CB mechanisms, stereo chemistry and orientation in E2 eliminations, pyrolytic elimination reactions, Eliminations Vs Substitution reactions. Esterification and hydrolysis mechanism

UNIT- III NAMED REACTIONS AND REAGENTS

a) Aldol, perkin, Benzoin, Cannizaro, Wittig, Grignard, Reformatsky reaction, Hydroboration, Openauer oxidation, Clemmensen reduction, Meerwein-pondorf-verley reduction, stark-enamine reactions, Michael addition, Mannich reaction, Diels-Alder reaction.

b) Reagents in organic synthesis
   Anhydrous $AlCl_3$, Borantrifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexyl carbodimide, leadtetraacetate.

UNIT-IV: ORGANOMETALLIC REAGENTS

(a) Preparation & Reactivity of Organomegnesium, Organolithium, Organozinc. Organo copper reagents.

(b) Metal mediated cross coupling reactions- Suzuki, Heck, Stille, Sonogishira, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

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CHEM-203: PAPER-III PHYSICAL CHEMISTRY –II

UNIT - I: THERMODYNAMICS – II

Statistical thermodynamics: Partial molar properties: their significance and determination of partial molar properties, fugacity and its determination. Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and micro- canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, Gibbs-Duhem equation, calculation of thermodynamic properties in terms of partition functions, Entropy of monoatomic gases (Sackur-Tetrade equation).

UNIT -II:CHEMICAL KINETICS – II

A)Homogeneous catalysis. Mechanism of catalysis. Equilibrium treatment. Steady state treatment. Acid base catalysis: Mechanism of acid base catalysis. Catalysis by enzymes. Influence of P^H. Michaelis Menten law. Influence of temperature. Examples. Decomposition of acetaldehyde catalysed by Iodine. Catalysed decomposition of hydrogen peroxide.

B)Free radicals in chemical reactions. Hydrogen oxygen reaction. Upper and lower explosion limits. Heterogeneous reactions. Bimolecular reactions. Adsorption. Langmuir adsorption isotherm. Electronic theories of chemisorption and heterogeneous catalysis.

C)Introduction to enzyme catalysis. Michaelis - Menten Kinetics – Effect of pH and effect of temperature on the rates of enzyme reactions.

UNIT -III: ELECTRO CHEMISTRY – II

A)Concept of activity and activity coefficient of an electrolyte. The mean ionic activity coefficient. Calculation of mean ionic activity coefficients. Debye Huckel theory of solutions. Debye Huckel Limiting law and its verification.

B) Electrode polarization-Decomposition potential and over voltage. Influence of C.D. on over voltage. Influence of P^H on over voltage, influence of temperature on over voltage-Theories of over-voltage. Hydrogen over-voltage.

C)Polarography**:** Theory, classification, principle, Instrumentation of Polarography, DME, HMDE diffusion current, Ilkovic equation, DC-Polarography, AC-Polarography, Controlled Potential Electrolysis, Millicoulometry, Equation for half-wave potentials, for reversible system when oxidant alone, reductant alone and both are present.

UNIT-IV: QUANTUM CHEMISTRY

Operators algebra- Commutation of operators, linear operators. Complex functions. Hamiltonian operators. Operators delta and delta square eigen functions and eigen values. Degeneracy . linear combination of eigen functions of an operator, well behaved functions. Normalized and orthogonal functions. Postulates of quantum mechanics. Physical significance of wave functions, observables and operators. Measurability of properties, average value of observable, time dependent and time independent schrodinger equation. Applications of schrodinger wave equations-particle 1-Dimensional and 3-Dimensional box, harmonic oscillator and rigid rotor

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CHEM-OC: 204: ENVIRONMENTAL CHEMISTRY-II (OPEN ELECTIVE)

UNIT: I: HYDROSPHERE

UNIT: II: ATMOSPHERE

UNIT: III: ENVIRONMENTAL TOXICOLOGY AND GREEN CHEMISTRY

UNIT: IV: ENVIRONMENTAL MONITORING METHODS

UNIT: I: HYDROSPHERE: 15 Hours

Introduction to Chemical composition of Environment- Bio distribution of elements Chemical composition of water bodies- lakes, streams, rivers and wet lands, Hydrological cycle. Aquatic pollution, inorganic, organic pesticides, agricultural, industrial and sewage, detergents. oil spills and oil pollutants, Water quality parameters,- DO, COD, BOD. Solids, metals, Contents of Chloride, sulphate, phosphate nitrate and micro organisms. Analytical methods of measuring BOD, DO, COD, Metals (As, Cr, Cd, Hg, Pb, Se) residual chloride and chlorine demand. Purification and treatment of water.

UNIT: II: ATMOSPHERE: 15 Hours

Chemical composition of Atmosphere- particles, ions and radicals and their formation, Chemical and photochemical reactions in atmosphere, smog formation, Oxides of N,C,S and their effects, pollution by chemicals, petroleum and minerals, chlorofuorocarbons, Green House effect, Chemical reaction in ozone depletion, Acid rain, Analytical methods for measuring air pollutants, Air pollution monitoring. Air pollution control methods.

UNIT: III: ENVIRONMENTAL TOXICOLOGY AND

GREENCHEMISTRY: 15 Hours

(a) Toxicological Chemistry: Introduction to toxicological chemistry, dose response relationship, relative toxicities. Teratogenesis, mutagenesis, carcinogenesis, Immune system effects, Health hazards, Toxic elements and elemental farms, Toxic inorganic compounds, Toxicology of organic compounds, Effect of Toxic chemicals on enzymes, biochemical effects of As, Cd, Hg and Oxides of Sulphur and nitrogen.

(b)Green Chemistry: Definition of Green Chemistry, Principles of Green Chemistry, Experimental systems. This measurement of greenness environmental factor, Historical approach, tools of green Chemistry, Catalysis

and bio-catalysis of Green Chemistry, examples of Green Chemistry, Pharmaceutical industry and Green Chemistry, Pesticides, Solvents, Green Chemistry, Sugar and distilleries, wastes and future trends in Green Chemistry.

UNIT: IV: ENVIRONMENTAL MONITORING METHODS:

(a) Monitoring of Air pollutants: Analysis of gaseous pollutants –SO_2, H_2S, NO, NO_X, NH_3, CO, CO_2, Ozone, organic gases and vapours. Continuous monitoring of air pollutants –principles, monitoring instruments, monitoring of SO_2, H2S, NO-NO_X, CO,CO_2,hydrocarbons ozone suspended particulate matter, chemical and photo chemical reactions in atmospheres.

(b) Monitoring of water pollutants: Analysis of polluted water samples using AAS, HPLC and ICP methods