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DETAILED SYLLABUS

FOR

DISTANCE EDUCATION

Post graduate degree Program

MASTER OF SCIENCE-CHEMISTRY

(M.SC.-CHEM.)

(YEARLY SYSTEM)

COURSE TITLE : MASTERS OF SCIENCE-CHEMSITRY
DURATION : TWO YEARS
MODE : YEARLY
TOTAL MARKS :

FIRST YEAR

Course Title	Paper Code	Marks				
		Theory		Practical		Total
		Internal	External	Internal	External	
Fundamentals of Inorganic Chemistry	MSCH/Y/110	40	60	NA	NA	100
Fundamentals of Organic Chemistry	MSCH/Y/120	40	60	NA	NA	100
Fundamentals of Physical Chemistry	MSCH/Y/130	40	60	NA	NA	100
Introduction to General Chemistry	MSCH/Y/140	40	60	NA	NA	100

FIRST YEAR

I) Fundamentals of Inorganic Chemistry Paper Code: MSCH/Y/110

I-01-Symmetry of molecules

Concept of Symmetry in Chemistry-Symmetry Operations and Symmetry Elements-rational axis of symmetry, plain of symmetry, rotation-reflex ion axis(improper axis) of symmetry, center of Inversion and Identity element. Molecular Point groups: assigning molecules to point groups, exercises on Groups.Degenerate and non-degenerate point groups-group multiplication tables. Symmetric Criteria for Optical Activity, symmetry and Dipole moment.

I-02-Inorganic Reaction Mechanisms

Energy Profile of reactions-reactivity of Metal Complexes: inert and liable complexes-kinetic applications of valence bond and Crystal field theories. Substitution Reaction: Nucleophilic substitution reactions of octahedral complexes. Dissociative and Associative Mechanism, acid hydrolysis. Factors affecting acid hydrolysis and base hydrolysis.SN1 .CB mechanism: direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal – ligand bond cleavage.

Redox reactions: electron transfer reactions , mechanism of one electron transfer reactions outer sphere type reactions, cross reactions and Marcus-Hush theory (Qualitative treatment), inner sphere type reactions-nature of bridging ligands.

I-03 Crystal Field Theory

Bonding in transition metal complexes interims of crystal field theory(CFT), d-orbital spitting in octahedral, compressed and Elongated octahedral, square pyramidal tetrahedral square planar, trigonal planar and linear complexes. Concept of weak and Strong ligand fields calculation of crystal field stabilization energy(CFSE) in six and four –coordinate complexes.high spin cross overs .Thermodynamic aspects of crystal field splitting –limitations of CFT, experimental evidences for metal ligand covalency.Russel Saunders-coupling scheme-free ion terms. Ground terms with various dn configurations. Splitting D and F terms in octahedral and Tetrahedral crystal fields.

I-04 Metal-Ligand Equlibria-Metal ions in Biological Systems

Stepwise and overall formation constants and their inter-relations .trends in stepwise constants.factors effecting the stability of metal complexes with reference to the metal ion and ligand.Chelate effect and its thermodynamic origin. Pearson's theory of hard and soft acids and base and its applications. Determination of binary formation constants by pH-metric and spectrophotometric methods.Metal ions in biological systems :brief survey of role of metal ions in biological systems.Oxygen transport by hemoglobin, cooperativity.Geometric ,electronic and magnetic aspects of dioxygen binding.Electron transport by cytochromes. Nitrogenous and biological nitrogen fixation .Fixation of Co2 in photosynthesis.

I-05 Metal Carbonyls, Metal nitrosyls, Metal Clusters

Eighteen electron rule in metal carbonyls, Structure and Bonding in Cr(CO)5 , Ni(Co)4, Mn2 (Co)10, Fe2(Co)9, Co2(Co)8.Concept of back bonding and its evidence from bond lengths, stretching frequencies and force constant data. Metal Nitrosyls: Linear and bent terminal NO groups, Bridging NO Groups, bridging NO groups. Structural Aspects [Ir(ph3P)2(Co)(NO)Cl] and [Ru(Ph3P2)2(NO)2Cl].Steriochemical control of valence in [Co(diar)2(NO)(SCN)] and [Co(diar)2(NO)] complexes. Metal Clusters: Carbonyl clusters, low nuclearity (M3 and M4)clusters: Structural patterns in M3(CO)12 clusters(M=Fe, Ru, Os).M4(Co)12 clusters(M=Co, Rh, Ir).High nuclearity (M5, M6, M7 and M8) clusters. The capping rule-structural patterns in [Ni5(CO)12]2- , [Os5(CO)18]2-, Rh6(CO)16, Os6(CO)21, [Os8(CO)22]2-.Non carbonyl clusters: Major structural types in metal-metal multiple bonds-edge sharing bioctahedra, face sharing bioctahedra, tetragonal prismatic structure, trigonal ant prismatic structure and bonding in binuclear halides of Re(III) and octahedral halides of Mo (II).Classification and Carboranes on the basis of their skeletal structures, Wades rule, Closo, Nido, Arachano boranes and carboranes.

II) Fundamentals of Organic Chemistry Paper Code: MSCH/Y/120

Stereochemistry
Molecular Representations-Wedge Fisher, Newman and Saw-horse formulae, their description and inter convertibility.

Stereoisomerisms: Definition and Classification.
Molecular Symmetry and Chilarity: Symmetry operations(Cn, Ci and Sn).Point group Classification.Chiral point groups.Classification of Stereoisomerisms, based on symmetry and energy considerations, Disymmetric and Asymmmetric molecules.Molecules with a Single Chiral center, chiral manifestations(absence of reflection symmetry, optical activity, specific rotation etc.).Molecules with tetra coordinate chiral center(quartenary ammonium salts, N-oxides, silane derivatives, phosphines and sulphones).Molecules with tricoordinate chiral center (teriary amines, carbanions, phosphines and Sulphoxides).Concept of Dynamic anantiomerism.Configurational nomenclature: D, l and R, S- nomenclature.Determination of absolute configuration .Chemical correlation methods.Racemic modification , racemisation and resolution.Molecules with 2 or more chiral centers: Constitutionally asymmetric molecules(with dissimilar chiral carbons) and symmetrical molecules(with similar chiral carbons).Principles of axial chirality. Stereochemistry of allenes, spiranes and biphenyls.Geometrical isomerism in molecules having C=C, C=N, N=N and in cyclopropane, cyclobutane and cyclopentane.E, Ez nomenclature, Physical , spectral and chemical methods of determining the configuration.

Reaction Mechanisms
Brief review of the electronic effects in organic molecules.Nucleophlic substitution reactions at saturated carbon.Classification- SN1 and SN2 reactions based on kinetics and molecularity.Mechanism and stereochemistry of SN1and SN2 reactions.Factors affecting the rate of SN1 and SN2 reactions(such as substate structure, nature of nucleophile, nucleofuse and solvent).SN1 mechanism, mention of S,SN1 and SN2 mechanisms.Addition reactions of C=C: Addition involving symmetrical and unsymmetrical reagents.Addition of hydrogen halides to alkenes:regioselctivity.Addition of water, sulphuric acidhypohalous acids, hydroboration as example of functional group modifications and mechanism of reactions.Addition of halogens mechanism, H-NMR evidence for halonium intermediacy, stereospecific nature of these reactions Syn addition of reagents like borohydrides, potassium permagnate, osmium tetroxide, ozone.Epoxidation and hydrolysis of epoxides as example of anti addition.Electrophylic aromatic substitution reactions: general mechanism, complex and sigma intermediates.halogenation , nitration , sulfonation Fridel-Crafts alkylation and acylation. Mechanisms. Orientation in mono substituted and disubstituted benzene derivatives, effect of substituents, explanation based on the stability of sigma complex intermediates.
Theory of Aromaticity, benzenoids and non-benzenoidsAromatic character of cyclic conjugated polymers, Huckle's (4n+2)- pi electron rule and its limitations.Criag's rule.Classification of the cyclic conjugated hydrocarbons-alternate and non-alternate.Benzenoids and non-benzenoids aromatic compounds containing 2, 6 and 10 electron systems viz cyclopropenyl cations and cyclopropenones , Cyclopentadienide anions and Ferrocene as an example of mettalocenes.Cycloheptatrienyl cations and cycloheptatetrienone .Azulenes.

Biopolymers
Introduction to biopolymers, brief survey of their importance Carbohydrates: determination of configuration in (+)-glucose and (-)-fructose, their cyclic and conformation structures, conformation formulae(writing only) of D-ribose and 2,D-deoxyribose.Structure elucidation of sucrose.Conformational structure(writing only)of sucrose, maltose.

Proteins: synthesis of aspartic acid, cystine, proline, tryptophan, ornithine.Aminoacid sequence determination in polypeptide synthesis.Classification of proteins, secondary and tertiary structure of proteins.

Heterocyclic
Importance of hetrocyclic compounds, nomenclature, pi-excessive and pi-deficient systems.
Bicyclic ring systems derived from furan, pyrrole and thiophene Important synthetic methods and electrophilic substitution reaction of indole and benzofuran.Six membered heterocyclics having one hetero atom –pyridine.Important synthetic methods and substitution reactions

Tricyclic ring systems: carbazole and acridine.Important methods of synthesis and properties.
Bicyclic ring systems derived from pyridine:quinoline and isoquinoline.Important synthetic methods, substitution reactions and oxidative ring clevage reactions.

III) Fundamentals of Physical Chemistry Paper Code: MSCH/Y/130

P-01 Thermodynamics-1
Review of the First and Second Law of thermodynamics and their applications.The Concept of Entropy and Determination of Entropy changes.Third Law of Thermodynamics and Calculation of absolute entropies of the substances.Entropy of Mixing of Ideal gases.Concept and Significance of Helmholtz and Gibbs free energy .Concept of reversibility, irreversibility and equilibrium interims of Gibbs free energy changes.Variation of Gibbs free Energy change with temperature .Gibbs Helmholtz equation –its derivation , significance and verification.

P-02 Thermodynamics-2 and Electrochemistry
Variation of free energy change with temperature and pressure.Clapeyron equation and Clausius – Clapeyron equation.Concept of Fugacity, activity and the significance of Activity coefficient, partial molar free energy, Chemical potential and its variation with temperature and pressure.Gibb's Duhem equation –its derivation .Elector chemistry: Cell E.M.F.Experimental determination of cell E.M.F. Standard electrode potential –SOP and SRP.reference electrodes, SHE(Standard Hydrogen Electrode) and SCE (Saturated Calomel Electrode).Various types of elctrode.Thermodynamics of electrode potential –Nernst equation , its derivation .Chemical cells and concentration cells with and without transference .Determination of transport number, liquid junction potential and solubility product .Ph and its determination from EMF measurements.

P-03 Quantum Chemistry 1
Black body radiation-Failures of classical mechanisms Plank's Quantum Theory –Concept of Quantisation –derivation of Plank's Equation –wave particle duality, uncertainty principle.Introduction to quantum mechanics-Schrodinger wave equation and its derivation-significance of wave function , well behaved nature of wave functions- normalized and orthogonal wave functions.

P-04 Quantum Chemistry 2 and Chemical Bonding
Particle in a box, in one dimensional and three dimensional boxes discussion of results and concept of degeneracy-application to spectra of conjugated molecules.The problems of potential barrier of infinite width(potential step).Wave equation for hydrogen atom and separation of variables-discussion of radial and angular wave functions(mathematical solving not included).Many electron systems and approximate methods in quantum mechanics-variation theorem(proof not necessary).The variation methods and construction of molecular orbitals.Outline of valance bond (VB)and molecular orbital(MO)approaches-Methods of linear combination of Atomic orbitals (LCAO).Trial wave functions and energies for H2+ molecule ion by MO method>Molecular orbitals and electronic configurations of homonuclear diatomic molecules and heteronuclear diatom molecules(LiH, HF, NO and CO).

P-05 Chemical Kinetics and Photo Chemistry
Theories of Reactionates-Collision theory, Elementary ideas of transition state theory (no derivation) and thermodynamic formulation of reaction rates-unimolecular reactions and Lindamann's Theory.Linear free energy relationships-Hammet and Taft equations and their applications.Acid-base Catalysis-protolytic and protropic mechanism-mechanism and ester hydrolysis –and introduction to enzyme catalysisComplex reactions-opposing-parallel and consecutive reaction with examples(first order type).Chain reactions-general characteristics, study state treatment-chain length.Examples:H2-Br2,H2 –Cl2 reactions, derivation of rate law.Photo Chemistry: Electronically excited molecules-singlet and triplet states, photo physical processes-Jablonski diagram.radiationless Transitions- internal conve4rsions and intersystem crossing-Fluorescence emission-phosphorescence emission – quantum yield and its determination reaction with high and low quantum yields. Experimental setup for carrying out photochemical reactions.

IV) Introduction to General Chemistry Paper Code: MSCH/Y/140

G-01 Mathematics-1

Function and Graphs; Interrelation of Cartesian , planar and Spherical polar coordinates. Equation of a Straight line-meaning of slope and Intercept, one point and two point equations. Equation of circle, parabola and hyperbola –their graphical representations.Differential Calculus: Differential coefficient , differentiation of algebraic, exponential logarithmic, trigonometric and composite functions .Product and Quotient formulae.maxima and Minima.Partial differentiation and meaning of total derivative .

G-02 Mathematics-2

Integration: Standard formulae-Integration by parts, definite integrals, areas, Differential equations: First order differential equation and their solutions (elementary treatment)-exact differentials and test for exactners

G-03 Computer Science

Introduction to computers and computer languages .types and Classifications of Computers .Input and output devices.Central processing unit.A brief introduction of the software .Algorithms and flowcharts.Elements of BASIC programming language.Expression in BASIC .Input and output specifications. IG-THEN and GOTO statements .DO loops, FOR-TO and NEXT statements.Library functions.Subroutine and Function programs, Subscripted variables and dimension statements.Writing of simple BASIC and FORTRAN programs for:Summation of seriesLeast square fitting of X-Y data to a straight line.Stability constant of a Binary metal complex.Introduction to C –language. C language instructions.C-language functions.printf(), scanf(), gets(), puts(),.Simple source program in C.Steps in testing the source program .Writing in C- language programs for:Roots of a Quadratic equationsDetermination of the first order rate constant from kinetic dataDissociation constant if acetic acidTo determine the value of 2×2 and 3×3 determinants

G-04 Spectroscopy-1 (Rotational and Vibrational Spectra)

Rotational Spectra: Rotational spectra of diatomic molecules-rotational energy levels-selection rules for rotational spectra-calculation of moment of inertia and bond distance of diatomic molecules.Vibrational Spectra: Vibrational energy levels of diatomic molecules-rotational energy levels-selection rules for vibrational spectra –calculation of force constant-anhormonic nature of vibrations: vibration -rotational Spectra of diatomic molecules-vibration of polyatomic molecules, normal modes of vibration-concept of group frequencies.Characteristics of vibrational frequencies of functional groups-structural and stereochemical effects on the absorption pattern in carbonyl group-absorption pattern in substituted benzenes, cis-trans –isomerism,hydrogen bonding, tautomerism and conformational analysis, Application to metal ligand bonding modes involving monodentate and bidentate ligands.

G-05 Spectroscopy-II (NMR Spectra I)

Magnetic susceptibility, Principals of magnetic resonance, Magnetic moment and Spin angular momentum, Larmor frequency.Proton magnetic resonance.Insrumentation , shielding constants, chemical shifts, shielding and deshielding mechanisms , spin coupling and Coupling constants. Applications of PMR spectroscopy in structure determination .Elecronegativity, keto enol tautomerism , proton exchange in alcohols , amines and Carboxylic acids, hydrogen bonding, C-N rotation.Reaction mechanisms, evidence for cyclic bromonium ion .Chemical shifts in aromatic elecrophilic substitution and nucleophilic substiution , carbocations, carbanions and in the conformational studies of cyclohexane.

G-06 Spectroscopy-III(NMR Spectra II)

Introduction to second order spectra , different methods to simplify the complex spectra (qualitative treatment only).Double resonance techniques, deuterium exchange , chemical shift reagents and nuclear overhauser effects(NOE)NMR in paramagnetic compounds. PMR spectrum of tris(4, 6-dimethyl phenonethroline)Cobalt(II).Metal hydride complexes.Acetylacetone complexes.Fluxional molecules.