M.Sc. Chemistry

Choice Based Credit System

Four Semester Course

Course Structure

SEMESTER I

(Session 2015-2017)

Code	Course	C/E	L	T	P	Credit
MCH-101	Inorganic Chemistry-I	Core	3	0	0	3
MCH-102	Organic Chemistry-I	Core	3	0	0	3
MCH-103	Physical Chemistry-I	Core	3	0	0	3
MCH-104	Group Theory & Spectroscopy-I	Core	3	0	0	3
MCH-105	Lab-1(Inorganic Chemistry)	Core	0	0	3	2
MCH-106	Lab-2(Organic Chemistry)	Core	0	0	3	2
MCH-107	Lab-3(Physical Chemistry)	Core	0	0	3	2
MCH-108	Seminar	Core	0	0	1	1
MCH-109	Assignment	Core	0	0	1	1
	Total valid credits					**20**
MCH-110	Comprehensive Viva-voce	virtual credit				4

Total Credit Value: #20+4 (virtual credit)

SEMESTER I

Paper-l

MCH-101: lNORGANIC CHEMISTRY-1

Unit - l

Stereochemistry and Bonding in Main Group Compounds

Valence shell electron pair repulsion (VSEPR) theory and its applications, Walsh diagram (triatomic molecules), dл-pл bond, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules such as Atomic inversion, Berry pseudoration, Nucleophilic displacement, free radical mechanisms.

Unit - ll

Metal Ligand bonding

Limitation of crystal field Theory, Jahn -Teller effect, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes

Unit - lll

Metal -Ligand Equilibrium in Solution

Stepwise and overall formation constants and their relationship, trends in stepwise constant, 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 Spectrometry.

Unit - IV

Reaction Mechanism of Transition Metal Complexes - I

Energy Profile of a reaction, reactivity of metal complex, 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, anion reactions, reactions without metal ligand bond cleavage. Substitution reaction in square planer complexes, the trans effect, Mechanism of substitution reactions.

Unit-V

Reaction Mechanism of Transition Metal Complexes - II and HSAB theory

Redox reaction, Electron transfer reaction, mechanism of one electron transfer reaction, outer and inner sphere type reactions, cross reactions and Marcus - Hush theory, HSAB principle, Theoretical basis of hardness and softness, Lewis - acid base reactivity approximation; donar acceptor numbers, E and C equation : applications of HSAB concept.

Books suggested

1. Advanced Inorganic Chemistry, F. A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of Elements. N. N. Greenwood and A. Earnshow, Pergamon
4. Inorganic Electronic Spectroscopy, A.B. P. Lever, Elsevier.
5. Comprehensive Co-ordination Chemistry eds., G. Wilkinson, R.D. Gillars and J. A. Mc clevetry, Pergamon.
6. Inorganic Chemistry, D. F. Shriver & P.W. Atkins, Oxford University Press 3rd 1999.
7. Inorganic Chemistry by A.G.Sharpe. Addition Wesley England 3rd 1992
8. Inorganic Chemistry G.L.Misseler and D. A. Tarr Pearson Education, 2009.

Paper – II

MCH – 102 : ORGANIC CHEMISTRY-I

Unit - I

Nature of Bonding in Organic Molecules

Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, Energy level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, catenanes and rotaxanes.

Unit - II

Stereochemistry

Strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in absence of chiral carbon in biphenyls, allenes and spiranes, Chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit - III

Confomational analysis and Linear free energy relationship

Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and Linear free energy relationship, substituents and reaction constants, Taft equation.

Unit - IV

Reaction Mechanism : Structure and Reactivity

Types of mechanism, types of reactions, thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond’s

Postulate, Curtin-hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopic effects.

Unit - V

Aliphatic Nucleophilic Substituition

The SN2, SN1, mixed SN1 and SN2 and SEI mechanism. The neighbouring group mechanism. neighbouring group participation by pi and sigma bonds, anchimeric assistance**.** Classical and non classical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SNi mechanism. Nucleophilic substitution at an allylic, trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophiles, regioselectivity.

Book Suggested

1. Advanced Organic Chemistry - Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry,_C.K. Ingold, Comell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice - Hall.
6. Modern Organic Reactions, HO. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blaclcie Academic & Professionls.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S. M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age lnternational.

Paper - III

MCH - 103: PHYSICAL CHEMISTRY-1

Unit - I

Introduction to Exact Quantum Mechanical Results

Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom.

Unit - II

Approximate methods

The variation theorm, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Molecular Orbital Theory

Huckel theory of conjugated systems bond and charge density calculation. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Huckel theory.

Unit - III

Angular Momentum

Ordinary Angular Momentum, generalized angular momentum, eigen fucntions for Angular Momentum, eigenvalues of Angular Momentum, operator using ladder operators addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

Unit - IV

Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, Partial molar volume and Partial molar heat content and their significance, Determinations of their quantities. Concents of fugacity and determination of fugacity. Non-ideal

systems : Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transition.

Unit - V

Statistical Thermodynamics

Concept of distribution, thermodynamics probability and most probable distribution. Ensenble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles. Corresponding distribution laws (using Lagrange's method of undeteremined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions. Calculation of thermodynamics probability in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and application to metal. Bose-Einstein statistics distribution Law and application to helium.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra. Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Couison's Valence, R.Mc Weepy, ELBS.
5. Chemical Kinetic. K. J. Laidler, MoGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacose, Mc Milian.
7. Micelies, Theoretical and Applied Aspects V.MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol. ll J.O.M Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Bastern.
10. Introduction to Quamum Chemistry-R.K. Prasad New Age Publication.

Paper – IV
MCH – 104: Group Theory & Spectroscopy-I
Unit – I

Symmetry and Group theory in Chemistry

Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes.Point symmetry group. Schoenflies symbols, representations of groups by matrices (representation for the C_n,C_{nv},C_{nh}, and D_{nh} group to be worked out explicity). Character of a representation. The 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_20 molecule.

Unit - II

Microwave Spectroscopy

Electromagnetic spectrum, Quantization of energy, Interaction of electromagnetic radiation with molecular system, Doppler broadening. Pure rotational Spectra: Instrumentation, rigid rotator model, effect of isotopic substitution on the transition frequencies, non-rigid rotator model, Stark effect, Application of rotational spectra to the calculation of bond length of diatomic molecules.

Unit - III

Infrared-Spectroscopy

Review of linear harmonic oscillator,Vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibration, normal co-ordination analysis.

Unit - IV

Raman Spectroscopy

Classical and quantum theories of Raman effect. Vibration and vibrational -rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman Spectroscopy , coherent anti stokes Raman Spectroscopy (CARS).

Unit - V

Electronic Spectroscopy

Energy levels, molecular orbitals, vibronic transition, vibrational progressions and geometry of the excited sates, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Photoelectron Spectroscopy

Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy-basic idea.

Books suggested

1. Modern Spectroscopy, .l.M. Hollas, John Viley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and FL. Ho, Wiley Interscience.
3. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R,V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F .A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill. ,
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper &Row.

PRACTICALS

(Duration : 6 - 8 hrs in each branch)
Practical examination shall be conducted separately for each branch.

MCH-105: Inorganic Chemistry **M.M. : 100**

Quantitative Analysis	30
Preparation	20
Viva	10
Internal assessment	40

Quantitative Analysis :

Separation and determination of two metal ions Ag-Ba, Cu-Ni, Ni-Zn etc., involving volumetric and gravimetric methods.

Preparations :

Preparations of selected inorganic compounds and their studies by I.R. electronic spectra, Mossbauer, E.S.R. and magnetic susceptibility measurements.

1. $VO(acac)_2$
2. $TiO(C_9H_8NO)_2H_2O$
3. cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. $Ni(acac)_2$
6. $K_3[Fe(C_2O_4)_3]$
7. Prussian Blue, Turnbull's Blue.

MCH-106: Organic Chemistry **M.M. : 100**

Qualitative Analysis	50
Viva	10
Internal Assessment	40

Qualitative analysis

Separation, Purification and Identification of Compounds of binary and ternary mixture using following solvents:-

(i) Saturated Solution of Sodium Bicarbonate
(ii) Water
(iii) Sodium hydroxide
(iv) HCl
(v) Organic Solvent

MCH-107: Physical Chemistry **M.M. : 100**

Error Analysis and statistical Data Analysis	10
Chemical Kinetics	20
Solution	20
Viva	10
Internal Assessment	40

Error Analysis and statistical Data Analysis :

Errors and type of errors, minimization of errors, distribution curves, precision, accuracy and combination; statistical treatment of error analysis, students‘ t’ test, null hypothesis, rejection criteria. F &Q test; linear regression analysis, curve fittingm. Calibration of volumetric apparatus, burette, pipette, and standard flask Adsorption to study surface tension-concentration relationship for solutions (Gibbs Equilibria.

i. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).

ii. Determination of glass transition temperature of given salt (e.g. CaCl2) Conductometrically.
iii. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water)

Chemical Kinetics :

I. Determination of the effects of (a) Change of temperature, (b) Change of concentration of reactant and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reaction.

II. Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.

III. Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide, study the kinetics as an iodine clock reactions.

IV. Flowing clock reactions (Ref. Experiments in physical Chemistry by showmaker)

V. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ions is oxidized by persulphate ion).

VI. Oscillatory reaction.

Solution :

I. Determination of molecular weight of non - volatile and electrolyte / electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
II. Determination of degree of dissociation of weak electrolyte and to study the deviation from ideal behavior that occurs with a strong electrolyte.