FATIMA MATA NATIONAL COLLEGE
KOLLAM, KERALA
(Autonomous)

MSc Degree in Chemistry

(Semester System)

Course Structure and Syllabus

Board of Studies in Chemistry

March 2015

PREAMBLE

The syllabus of M.Sc programme in Chemistry offered under Semester system has been revised and effective from 2015 admission. There is one independent PG programme in Chemistry, namely M.Sc. Programme in Branch III –Chemistry. This PG programme shall extend over a period of two academic years comprising of four semesters, each of 450 hours in 18 weeks duration. The syllabi and scheme of examinations of this programmes is detailed below.

M.Sc. PROGRAMME IN BRANCH III - CHEMISTRY

(Revised syllabus under semester system with effect from 2015 admission)

SYLLABUS AND SCHEME OF EXAMINATION

Course No. and Title	Hours per week		Duration of ESA in hours	Marks for CA	Marks for ESA	Total marks
	L	P				
SEMESTER I*						
15PCH 11 Inorganic Chemistry I	5		3	30	70	100
15PCH 12 Organic Chemistry I	5		3	30	70	100
15PCH 13 Physical Chemistry I	5		3	30	70	100
15PCH 14 Inorganic Practicals I		3	(To be continued in Semester II)			
15PCH 15 Organic Practicals I		3	(To be continued in Semester II)			
15PCH 16 Physical Practicals I		4	(To be continued in Semester II)			
			Total marks for semester 1			300
*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)						
SEMESTER II*						
15PCH 21 Inorganic Chemistry II	5		3	30	70	100
15PCH 22 Organic Chemistry II	5		3	30	70	100
15PCH 23 Physical Chemistry II	5		3	30	70	100
15PCH 14 Inorganic Practicals I		3	6	30	70	100
15PCH 15 Organic Practicals I		3	6	30	70	100
15PCH 16 Physical Practicals I		4	6	30	70	100
	Total marks for Semester II					600
*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)						

SEMESTER III*

15PCH 31 Inorganic Chemistry III	5		3	30	70	100
15PCH 32 Organic Chemistry III	5		3	30	70	100
15PCH 33 Physical Chemistry III	5		3	30	70	100
15PCH 34 Inorganic Practicals II		3	(To be continued in Semester IV)			
15PCH 35 Organic Practicals II		3	(To be continued in Semester IV)			
15PCH 36 Physical Practicals II		4	(To be continued in Semester IV)			
			Total marks for semester III			300
*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)						
SEMESTER IV*						
15PCH 41(a) Advanced Inorganic Chemistry**						
15PCH 41(b) Advanced Organic Chemistry**	15		3	30	70	100
15PCH 41 (c) Advanced Physical Chemistry**						
15PCH 34 Inorganic Practicals II		3	6	30	70	100
15PCH 35 Organic Practicals II		3	6	30	70	100
15PCH 36 Physical Practicals II		4	6	30	70	100
15PCH 42(a) Dissertation					90	90
15PCH 42(b) Visit to R & D Centre					10	10
15PCH 43 Comprehensive viva-voce					100	100
		Total marks for Semester IV				600
	Grand total (for semesters I-IV)					1800
*Distribution of teaching hours/week: Theory- 15 hours, 10 hours for discussion on project (1 hour for Seminar)						
**Each student has to choose either (a), (b), (c) as elective in accordance with the Dissertation chosen.						

M.Sc. PROGRAMME IN BRANCH III - CHEMISTRY

(Revised syllabus under Semester System w.e.f. 2015 Admission)

SEMESTER I

15PCH 11 INORGANIC CHEMISTRY - I

Total 90 h

Unit I Noble gases, halogens, isopoly and heteropoly acids 18 h

Noble gas compounds: Preparation, properties, structure and bonding. Halogens in positive oxidation states. Preparation, properties, structure, bonding and uses of inter halogen compounds, pseudo halogens, poly halide ions. Astatine: Synthesis, stability and properties.

Preparation, properties and structure of isopoly and heteropoly acids of Mo and W. Classification, preparation, properties and structure of borides, carbides, nitrides and silicides. Classification and structure of silicates. Properties and structure of aluminosilicates and zeolites. Preparation, properties and applications of silicones.

Unit II Coordination chemistry-I: Theories of metal complexes 18 h

Types of ligands and complexes. Isomerism: Geometrical, optical and structural isomerism. Stability of complex ions in aqueous solutions: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Trends in stepwise constants. Determination of stability constants: spectrophotometric, polarographic and potentiometric methods. Stability of chelates. Thermodynamic explanation, macrocyclic effects.

Crystal field theory: Splitting of d orbitals in octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields. Jahn-Teller theorem, dynamicstatic - evidence for JT effect. Crystal field stabilization energy (CFSE) and its calculations. Octahedral Site Stabilization Energy. Thermodynamic effects of CFSE. Factors affecting the splitting parameter. Spectrochemical series. Ligand field theory. Molecular orbital theory. Sigma and pi bondings in complexes. MO diagrams of octahedral complexes with and without pi bonds. Effect of pi bond on the stability of sigma bond. Nephelauxetic effect. Critical comparison of the three theories.

Unit III Coordination chemistry-II:

Spectral and magnetic properties of transition and inner transition metal complexes

18 h

Electronic spectra of transition metal complexes- Term symbols of d^n system, Racah parameters, splitting of terms in octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling. Interpretation of electronic spectra of complexes- Orgel diagrams, Tanabe-Sugano diagrams, Calculation of Dq, B and β (Nephelauxetic ratio) values, charge transfer spectra. Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy's method for the determination of magnetic moment of complexes, spin only magnetic moment.

Lanthanides and Actinides: Electronic configuration, Spectral and magnetic properties.

Application of magnetic measurements in the determination of structure of transition and inner transition metal complexes.

Unit IV Nanomaterials **18 h**

General introduction to nanomaterials and emergence of nanotechnology, Moore‟s law, synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum. Techniques of synthesis- electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films-chemical vapour deposition and atomic layer deposition techniques.

Elementary idea of characterization of nanomaterials using XRD powder, Neutron diffraction, Electron diffraction, XPS, DLS, TEM, AFM, SEM and STM techniques. Flame emission and atomic absorption spectrometry.

Diversity in nanosystems: self assembled monolayers on gold-growth process and phase transitions. Gas phase clusters- formation, detection and analysis. Quantum dots-preparation, characterization and applications.

Unit V Chemistry of natural environmental processes **18 h**.

The chemistry of processes in atmosphere: Composition of the atmosphere: Automobile

pollutants and the catalytic converter. Photochemical smog. Chemistry of the stratosphere. Catalytic destruction of ozone. Depletion of the protective ozone layer. Effects of air pollutants on the human health. Atmospheric Radiation and Photochemistry: Radiation – Terrestrial and solar radiation – Energy balance for Earth and Atmosphere – Radiative flux – Actinic flux; Photochemistry – Absorption of radiation by atmospheric gases – Absorption by O_2 and O_3 – Photolysis rate as a function of altitude – Photodissociation of O_3, NO_2.

The Chemistry of processes in hydrosphere: The hydrologic cycle. Cycling and purification. The unique properties of water. Acid base properties. CO_2 in water. Alkalinity. O_2 consuming waste.

The chemistry of processes in Lithosphere: Redox status in soil. pE/pH predominance diagrams for redox sensitive elements. Acidity in soil materials.Acid neutralization capacity and the quantification of the soil acidity. Ion speciation in soil solution. Quantitative aspects of ion speciation. Cation exchange capacity and exchange phase composition.

References

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2. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", John Wiley and Sons.
3. J. E. Huheey , "Inorganic Chemistry- Principles of Structure and Reactivity" , Harper Collins College Publishing
4. K. F. Purcell and J. C. Kotz, "Inorganic Chemistry" , Saunders.
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7. A. I. Vogel, "A Text Book of Quantitative Inorganic Analysis" , Longman.
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9. Geoffrey A. Ozin and Andre C. Arsenault, "A Chemical approach to Nanomaterials" RSC Publishing.

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12. K. J. Klabunde (Ed.), “Nanoscale Materials in Chemistry” John Wiley and Sons.
13. C.P. Poole Jr. and J. Owens,“ Introduction to Nanotechnology” Wiley India.
14. James E. Girard, “Principles of Environmental Chemistry” Jones and Bartlett Publishers, Inc.
15. H.V. Jadhav, “Elements of Environmental Chemistry” Himalaya Publishing House.
16. M. Essington “Soil and Water Chemistry” CRC Press.
17. S. Cotton, “Lanthanides and Actinides” , Macmillan.
18. J. C. Bailer, “Chemistry of Coordination Compounds” , Reinhold.
19. Figgins and Hitchman, “Ligand Field Theory and its Applications” , Wiley-VCH.
20. D. Sutton, “Electronic Spectra of Transition Metal Complexes” , McGraw Hill.
21. C. E. Houecroft, “Cluster Molecules of p- block elements”, Oxford Scientific Publication.

15PCH 12 ORGANIC CHEMISTRY - I

Total 90 h

Unit I Stereochemistry of organic compounds 18 h

Nomenclature of organic compounds, Fused polycyclic hydrocarbons, Bridged polycyclic hydrocarbons, Bridged fused systems, Spirocyclic hydrocarbon systems, Heterocyclic systems,Metal organic compounds.

Molecular chirality, stereochemical nomenclature, prostereoisomerism, stereotopicity and stereoprojections. Non-carbon chiral centres. Introduction to ORD, CD configuration and their application in assigning configuration and conformation. Octant and axial haloketone

rules. Cotton effect. Stereochemistry of nitrogen and phosphorus containing compounds. Atropisomerism and its designation. Stereoselectivity, enantiomeric excess and chiral separation methods. Conformational analysis of alkanes, cycloalkanes and biased systems. Effect of conformation on reactivity of cyclohexane and decalin derivatives. Chiral drugs.

Unit II Structure, reactivity and intermediates **18 h**

Electronic and steric effects. Influence of structural features on acidity, basicity and reactivity of organic compounds. Structure, formation and properties of carbens, nitrenes and arynes. Singlet and triplet carbenes, formation and reactions. Carbon radicals: Structure, formation and stability. Radical reactions, autoxidation and radical chain reactions. Structure, stability and formation of carbocations, carbanions. Arynes: Formation and structure. S_N1, S_NAr, benzyne and $S_{NR}1$ mechanism in aromatic nucleophilic substitution.Orientation effects of substituents in aromatic electrophilic substitutions.

Unit III. Substitution and elimination reactions **18 h**

Nucleophilic susbstitution at sp^3carbon, its mechanisms and stereochemical aspects. Effect of solvent, leaving group and substrate structure. S_{N1} , S_{N2}, S_N1^1, S_N2^1, S_Ni reactions. Neighbouring group participation. Non-classical carbocations. Elimination reactions leading to C=C ond formation and their mechanisms. E1, E2 and E1CB mechanisms. Stereoaspects of C=C bond formation. Effect of leaving group and substrate structure. Hoffmann and Saytzeff elimination. Cis elimination. Competition between S_{N1} and S_{N2} , E1and E2, Alkyl halides as survival compounds

Unit IV Reactivity of unsaturated systems **18 h**

Stereoaspects of the addition of X_2, HX, boranes and hydroxylation to C=C systems**.** Effect of substituents on the rate of additions. Cis and trans hydroxylation of cycloalkenes. Nucleophilic addition to activated C=C systems. Michael addition. Mechanism, with evidence of Aldol (normal, crossed and directed), Perkin, Stobbe, Knovenagel, Darzen, Reformatsky and benzoin condensations. Grignard, Cannizaro, Wittig and Wittig-Horner reactions. Mechanism and stereochemistry of addition to C=O systems. Cram‟s rule, Felkin-Anh model, Mechanism of esterification and ester hydrolysis. Structure of the transition state in the addition reactions.

Unit V Separation techniques **18 h**

Classification of chromatographic methods. Theory of chromatography. Applications of chromatographic methods. Adsorption and partition chromatography. Paper, thin layer and column chromatographic methods. Centrifugal TLC, LC, Pressure column chromatography, HPLC and GC. Column matrices. Detectors. Affinity and chiral separations using HPLC. Normal and ultra centrifugation. Gel and Capillary electrophoresis and their applications. Solvent extraction. Extraction using supercritical liquid CO_2, Craig‟s technique of iquid liquid extraction.

References

1. D. Hellwinkel, Systematic Nomenclature of Organic Chemistry, Springer international edition

2. D. Nasipuri, "Stereochemistry of Organic Compounds", Wiley Eastern.

3. Jonathan Clayden, Nick Greeves, and Stuart Warren , Organic Chemistry, OUP.

4.P.S. Kalsi, Sterochemistry, Conformation and Mechanism, New age.

5. Paula Yurkanis Bruice, " Organic Chemistry", Third Edition, Pearson Education.

6. P. Sykes, " A Guide Book to Mechanism in Organic Chemistry", Longman.

7. S. N. Issacs, " Physical Organic Chemistry", Longman.

8. M.B. Smith, March‟s Advanced Organic Chemistry" 5th Edn, Wiley.

9. F. A. Carey and R. S. Sunderg, Advanced Organic Chemistry, part A and B", Kluwer, 4th Edn.

10. M. A. Fox and J. K. Whitesell, " Organic Chemistry", 2nd Edn, Jones and Bartlett.

11. C. J. Moody and W. H. Whitham, " Reactive Intermediates", Oxford University Press.

12. D. A. Skoog, D. M. West and F. J. Holler, " Fundamentals of Analytical Chemistry", Saunders College Publishing.

13. D. J. Holme and H. Perk, " Analytical Biochemistry", Blackie.

14. I. L. Finar, " Organic Chemistry" Vol 2, Longman.

15. F. Carey, " Organic Chemistry" 5th Edn, Mc Graw Hill.

15PCH 13-PHYSICAL CHEMISTRY -I

Total 90 h

Unit I Quantum mechanics **18 h**

Experimental foundation of quantum mechanics- The black body radiation, Compton effect, photoelectric effect, atomic spectra. Failure of classical mechanics, need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences.

The postulates of quantum mechanics: Wave function postulate- wave function and its physical meaning, well behaved functions, boundary conditions, orthogonality and orthonormality. Operator postulate- Laplacian and linear operators. Angular momentum operators and commutators. Hamiltonian operator and its properties. Eigen value postulateeigen value equations and eigen functions. Expectation value postulate. Postulate of timedependent Shrodinger equation.

Application to simple systems: Solution of Schrodinger wave equation for a free particle, particle on a ring, particle in 1D box, particle in 3D box, separation of variables, degeneracy.

One dimensional Harmonic oscillator- Complete solution. Hermite polynomials, recursion formula, features of the wave functions.

Hydrogen like systems- wave equation in polar coordinate. Separation of variables. R, theta and phi equations. Solution of phi equation. Wave functions of hydrogen like systems. Orbital and radial functions. Radial distribution functions, angular functions and their plots.

Stern-Gerlach experiment. The postulate of spin. Spin orbitals. Many electron atoms. Qualitative idea of self consistant field method. The exclusion principle. Vector atom model. Spin-orbit coupling. Term symbols and explanation of spectral lines.

Unit II Molecular symmetry **18 h**

Symmetry and Character table: Symmetry elements and symmetry operation. Matrix representation of symmetry operations. Character of a matrix. Conditions for a set of elements to form a group. Point groups. Multiplication of operations. Group multiplication table. Similarity transformation and classification of symmetry operation, Matrix representation of point group. Reducible and Irreducible representations. The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v} and C_{2h} groups. Direct product representations.

Reduction formula, reduction of reducible representation to IRs. Transformation properties of atomic orbitals. Hybridisation: identification of atomic orbitals taking part in hybridisation of triangular planar, square planar, triagonal bipyramidal, square pyramidal and tetrahedral molecules. Molecular symmetry and optical activity.

Unit III Basics of thermodynamics . **18 h**

Phase equillibria: Criteria of Equillibrium. Derivation of phase rule Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases.

Three component systems: Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids. Two salts and water systems. Isothermal evaporation. Transition point and double salt formation.

Fugacity and Activity: Fugacity of gases, its determination. Variation of Fugacity with temperature and Pressure. Fugacity of liquids and solids. Fugacity of mixtures of gases. Lewis Randall rule. Fugacity in liquid mixtures. Activity and Activity coefficients. Determination of activity and activity coefficients of electrolytes and non electrolytes.

Reaction Isotherm and spontaneity of reaction. Variation of Equilibrium constant with temperature and pressure. Variation of standard free energy with temperature. Simultaneous equillibria and addition of free energies. Standard free energy of formation and its determination, Free energy functions.

Unit IV Chemical kinetics 18 h

Complex reactions, Reversible, Consecutive, Concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like H_2-Cl_2, H_2-Br_2, and decompositions of ethane , acetaldehyde and N_2O_5. Rice-Herzfeld mechanism, Potential energy surfaces-adiabatic and non adiabatic curve crossing processes. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelwood mechanism of chain reactions and explosion.

Kinetics of fast reactions: Relaxation method, relaxation spectrometry, flow method, shock method, fast mixing method, field jump method, pulse method Flash photolysis and NMR method.

Theories of Reaction rate: Arrhenius equation and its limitations, activation energy,

Collision theory and absolute reaction rate theory. Free energy of activation and volume of activation. Thermodynamic formulation of reaction rate. Effects of pressure and volume on the velocity of gas reaction.

Reactions in solution: Comparison between reactions in gas phase and in solution. Factors determining reaction rates in solution. Reaction between ions and influence of ionic strength. Primary and secondary kinetic salt effects. Influence of solvent on reaction rate. Significance of volume of activation. Hammet and Taft equation.

Photochemistry: Effect of radiation on the rate of reaction. Laws of photochemistry. Quantum yield. Photo chemical reactions of H_2-Cl_2, H_2-Br_2.

Unit V Solids, liquids and liquid crystals 18 h

Heat capacity of solids. Dulong and Petit's law, Kopp's law, Classical theory and its limitation. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. Limitations of Einstein's theory. The Debye theory, the electronic specific heat.

Liquid state: X-ray diffraction study of simple liquids and their structure. Oscillator theory of liquid state. Specific heat of liquids.

Liquid crystals: Mesomorphic state, types, examples and applications of liquid crystals. Theory of liquid crystals.

References

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2 D. A . McQuarrie, “Quantum Chemistry”, Viva Publishers.

3 M. W. Hanna, “Quantum Mechanics in Chemistry”, Benjamin.

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10 L.H.Hall, “Group theory and Chemistry”, McGrow Hill.

11 V. Ramakrishnan and M.S.Gopinathan,”Group Theory in Chemistry”, Vishal Publications.

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19 J.E.House,”Principles of Chemical Kinetics”, Elsevier.

20 J.Rajaram, J.C Kuriakose," Kinetics and Mechanisms of Chemical Transformations", McMillan.

21 C.Kalidas," Chemical Kinetic Methods: Principles of Fast reaction Techniques and Applications, New Age International.

22 K.K Rohatgi-Mukherjee, "Fundamentals of Photochemistry", New age International.

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15PCH 14 INORGANIC CHEMISTRY PRACTICALS -1

Total 125 h

1. Separation and identification of rare/less familiar cations such as Ti, W, Mo, Th, Zr, V, U and Li

2. Volumetric estimation using EDTA, ammonium vanadate, ceric sulphate etc.

3. Colorimetric/spectrophotomteric estimation of Cr, Fe, Mn, Ni, Cu etc.

4. Preparation of metal complexes: selection can be made from the following or any other from the existing literature.

i) $[Co(NH_3)_6]Cl_3$, (ii). $[Cu(NH_3)4]SO_4$ (iii) $K_3[Cr(C_2O_4)_3]$

iv). $K_3[Fe(C_2O_4)_3]$, v). Cis and trans isomers of $[Co(en)_2Cl_2]Cl$

iv). $[Cr(en)_3]Cl_3$

References

1. A. I. Vogel, "A Text Book of Quantitative Inorganic Analysis", Longman.

2. A. I. Vogel, "A Text Book of Qualitative Inorganic Analysis", Longman.

3. D.A. Skoog and D. M. West, "Analytical Chemistry: An Introduction", Saunders College Publishing.

4. W. G. Palmer, "Experimental Inorganic Chemistry", Cambridge University Press.

15PCH 15 ORGANIC PRACTICALS-1

Total 125 h

A . Separation and identification of organic compounds

1. Quantitative wet chemistry separation of a mixture of two components by solvent extraction

2. Purification of the separated samples by boiling and crystallization.

3. TLC of the purified samples along with the mixture in same TLC plates (if not possible use separate plates) and calculation of R_f values.

B. Separation of a mixture of by column chromatography

1) Malachite green and methylene blue 2) O-nitroaniline and p-nitroaniline.

C. Preparation of compounds by two stages.

TLC analysis of the products and original compound in the same plate and measurement of Rf values. Recording UV, IR, NMR and mass spectrum of synthesized compounds.

1) Acetanilide- p-nitroacetanilide p-nitroaniline

2) Methylbenzoate m-nitromethylbenzoate m-nitrobenzoic acid

3) Acetanilide- p-bromoacetanilide p-bromooaniline

E. Green Organic Chemistry experiments

1) Acetanilide- p-bromoacetanilide (KBr and CAN)

2) Benzophenone Benzopinacol (photoreduction)

References

1. B S Furniss, Vogels Text Book of Practical Organic Chemistry. Prentice Hall
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15PCH 16 PHYSICAL PRACTICALS -I

Total 125 h

1. Adsorption

Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal.

Determination of concentration of acetic/ oxalic acid.

2. Kinetics

Determination of rate constant of acid hydrolysis of methyl acetate.

Determination of Arrhenius parameters.

Determination of concentration of given acid.

Determination of rate constant of the saponification of ethyl acetate and evaluation of Arrhenius parameters.

Determination of rate constant of reaction between $K_2S_2O_8$ and KI.

Study the kinetics of iodination of acetone in acid medium.

3. Phase rule

Solid-liquid equilibria - Construction of phase diagram and determination of the composition of unknown mixture (naphthalene/biphenyl, naphthalene/benzophenone, naphthalene/diphenyl amine). Construction of phase diagram with congruent melting point -naphthalene/meta-dinitrobenzene

Partially miscible liquid pairs- CST of phenol-water system.

Effect of impurities (KCl/ NaCl/ succinic acid) on the miscibility temperature of phenol-water system and hence the concentration of given unknown solution.

Three component system- Construction of ternary phase diagram of acetic acid-chloroform-water system and hence the composition of given homogeneous mixture.

Construction of tie-line.

4. Distribution law

Distribution coefficient of iodine between CCl_4 and water

Distribution coefficient of benzoic acid between toluene and water.

Determination of the equilibrium constant of the reaction $KI+I_2 \rightarrow [KI_3]$ and hence the concentration of given KI.

Distribution coefficient of ammonia between chloroform and water.

Determination of equilibrium constant of copper- ammonia complex by partition method or coordination number of Cu^{2+} in copper-ammonia complex.

Determination of hydrolysis constant of anilinium hydrochloride.

5. Dilute solutions

Determination of K_f of solid solvent, molar mass of non-volatile solute, mass of solvent and composition of given solution (Solvent- Naphthalene/Biphenyl/ Benzophenone etc. Solute- Naphthalene/ Biphenyl/ Diphenylanmine etc)

Determination of vant Hoff"s factor for benzoic acid in Naphthalene.

Determination of atomicity of sulphur.

6. Transition temperature

Determination of K_T of salt hydrate, molar mass of solute, mass of salt hydrate and composition of given solution (Solvent- $Na_2S_2O_3.5H_2O/CH_3COONa.3H_2O$, Solutes glucose, sucrose, urea)

7. Thermochemistry

Determination of the concentration of given strongacid/alkali. Thermometric titration of NaOH vs standard HCl. Heat of displacement of Cu^{2+} by Zn.

Determination of the heat of ionisation of acetic acid.

References

1) V. D. Athawal, "Experimental Physical Chemistry", New Age International.

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8) D. P. Shoemaker, C. W. Garland & J. W. Nibler. "Experiments in Physical Chemistry", McGraw Hill.

SEMESTER II

15PCH 21 INORGANIC CHEMISTRY -II

Total 90 h

Unit I Sulphur, nitrogen, phosphorus and boron compounds 18 h

Sulphur-nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl S_xN_y compounds. S-N cations and anions. Other S-N compounds. Sulphur-posphorous compounds:

Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phophorous-nitrogen compounds: Phosphazines. Cylco and linear phosphazines. Other P-N compounds

Boron-nitrogen compounds: Borazine, substituted borazines and boron nitride. Boron hydrides: Reactions of diborane. Structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure. *Sytx* numbers. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. Structural study by NMR. Wade‟s rules. Carboranes. Metallocarboranes. Organoboron compounds and hydroboration.

Unit II Solid state chemistry **18 h**

Electronic structure of solids. Free electron theory, band theory. Refinements to simple band theory, k space and Brillouin zones. Conductors, insulators and semiconductors. Band structure of conductors, insulators and semiconductors and their applications. Colour in inorganic solids.

Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, zone refining, fractional crystallization, semiconductor devices, rectifier transistors, optical devices, photoconductors, photovoltaic cells, solar batteries.

Unit III Electrical and magnetic properties of solids 18 h

Conductivity of pure metals. Superconductivity. Photoconductivity. Photovoltaic effect, Dielectric properties. Dielectric materials. Ferroelectricity, pyroelectricity, piezoelectricity and ionic conductivity. Applications of ferro, piezo and pyroelectrics.

Magnetic properties of solids: Behaviour of substances in a magnetic field. Diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism and ferrimagnetism. Effect of temperature, Curie and Curie- Weiss laws. Magnetism of ferro and antiferromagnetic ordering. Super exchange. Lasers and their applications.

Unit IV Crystalline state **18 h**

Crystal systems and lattice types. Bravais lattices. Crystal symmetry. Introduction to point groups and space groups. Miller indices. Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP . Voids. Coordination number. Crystal binding: Molecular, covalent, metallic and hydrogen bonded crystals. X- Ray diffraction by crystals: Function of crystals. Transmission grating and reflection grating. Braggs equation. Diffraction methods: Powder, rotating crystal, oscillation and Weisenberg methods. Indexing and determination of lattice type and unit cell dimensions of cubic crystals.

Crystal defects: Perfect and imperfect crystals. Point, line and plane defects. Thermodynamics of Schottky and Frenkel defects. Colour centers in alkali halide crystals. Defect clusters. Extended defects: Crystallographic shear structure and stacking faults. Dislocations and crystal structure. Structure of compounds of AX (Zinc blende, Wurtzite) , AX_2 (Rutile, fluorite, antifluorite), A_mX_2 (Nickel arsenide), ABX_3 (Perosvskite, Ilmenite). Spinels. Inverse spinel structures.

Unit V Nuclear chemistry 18 h

Nuclear structure, mass and charge. Nuclear moments. Binding energy. Semiempirical mass equation. Stability rules. Magic numbers. Nuclear models: Shell, Liquid drop, Fermi gas, collective and optical models. Equation of radioactive decay and growth. Half life and average life. Radioactive equilibrium. Transient and secular equilibria. Nuclear reactions. Introduction, production of projectiles, nuclear reaction cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus. Nuclear reactions: Direct nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

Neutron capture cross section and critical size. Nuclear fission as a source of energy, Nuclear chain reacting systems. Principle of working of the reactors of nuclear power plants. Breeder reactor. Nuclear fusion reaction, stellar energy. Detection and measurement of radiation.

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15PCH 22 ORGANIC CHEMISTRY- II

Total 90 h

Unit I Molecular rearrangement and transformation reactions 18 h

Types of organic rearrangements. Anionic, cationotropic, prototropic, free radical, carbene, nitrene and long-range rearrangements. Mechanism with evidence of WagnerMeerwein, Pinacol, Demjanov, Hofmann, Curtius, Schmidt, Lossen, Beckmann, Wolf, Fries, Arylazo, Fischer-Hepp, Hofmann-Martius, Von-Richter, Orton, Bamberger, Smiles, Dienonephenol, Benzilic acid, Benzidine, Favorskii, Stevens, Wittig, Sommelet-Hauser, BayerVilliger, Hydroperoxide and borane rearrangements.

Unit II Aromaticity and symmetry controlled reactions 18 h

Aromaticity and antiaromaticity. Homo, hetero and non benzenoid aromatic systems. Aromaticity of annulenes, mesoionic compounds, metallocenes, cyclic carbocations, carbanions and fullerenes. Symmetry properties of MOs. Classification of pericyclic reactions. Mechanism and stereochemistry of electrocyclic, cycloaddition and sigmatropic reactions. Woodward- Hoffmann rules. FO, CD and Huckel-Mobius analysis of electrocyclic and cycloaddition reactions including biological cyclo additions. FO analysis of [I, j] and [3, 3] migrations. 1, 3- dipolar cycloaddition. Stereo aspects of Diels- Alder reaction and Cope re arrangement. Fluxinol molecules. Retro Diels- Alder, ene, cheletropic and cis elimination reactions and synthetic applications.

Unit III Organic photochemistry 18 h

Photochemical processes**.** Energy transfer, sensitization and quenching. Singlet and triplet states and their reactivity. Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Free radical reactions. Patterno-Buchi, Barton, photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions. Applications of photochemistry.

Unit IV Chemistry of natural products and biomolecules **18 h**

Introduction to primary and secondary metabolites in plants. Extraction methods of chemical constituents from plants, such as fractionation using solvents, specific extraction of alkaloids and supercritical fluid extraction. Characterizations of isolated compounds (terpenes, sterols, alkaloids, carbohydrates, flavonoids and poly phenols) by colour reactions and spray reagents. Biosynthesis of terpenes from mevalonic acid and sterols from squalene. Structure elucidation of ocimene monoterpene, classification of pigments, structure elucidation of β -carotene. Structural differences between a triterpene and a sterol. Synthesis of quercetin, synthesis of testosterone, androsterone, estrone and progesterone. Determination of carbon skeleton of alkaloids (Hofmann, Emde and Von Braun degradation methods). Structural elucidation of ephedrine, nicotine , atropine,hygrine.

Unit V Physical organic chemistry 18 h

Reactivity in relation to molecular structure and conformation. Steric effects. F strain. Ortho effect. Bond angle strain. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. Methods of determining reaction mechanisms. Phase transfer catalysis and its applications.

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15PCH 23 PHYSICAL CHEMISTRY -II

Total 90 h

Unit I Chemical Bonding 18 h

Approximate methods: Variation method- Variation theorem and its proof. Linear variation functions. Secular equations and secular determinants.

Perturbation method-Successive correction to an unperturbed problem. Detailed treatment of First order non-degenerate case only. LCAO-MO theory- MO theory of H_2^+ and H_2. Treatment of other homo diatomic molecules Li_2, Be_2, B_2, C_2, N_2, O_2 and F_2. MO treatment of hetero diatomic molecules LiH, CO, NO and HF. Spectroscopic term symbols for homo diatomic molecules.

Valance bond theory of H_2. Quantum mechanical treatment of SP, SP^2 and SP^3 Hybridisation. HMO theory of conjugated π-systems. Bond order and charge density calculations. Free valance. Application of HMO method to ethylene, allyl system, butadiene and benzene. Secondary bond forces: ion dipole, dipole-dipole, ion-induced dipole, London dispersion forces.

Unit II Spectroscopy -I 18 h

Microwave spectroscopy: Rotational spectrum, Intensity of spectral lines, calculation of inter nuclear distance. Non-rigid rotors and centrifugal distortion. Rotational spectra of polyatomic molecules-linear and symmetric top molecules. Introduction to instrumentation.

Vibrational Spectroscopy: Vibrational spectra of harmonic and anharmonic oscillator. Selection rules. Morse curve, fundamentals and overtones. Determination of force constant. Rotational fine structure, P,Q,R branches of spectra.

Vibrational spectra of polyatomic molecules: Normal modes, classification of vibrational modes into stretching (asymmetric, symmetric), bending, parallel and perpendicular vibrations. Finger print region and group frequencies. Introduction to FTIR and instrumentation.

Raman spectroscopy: Raman scattering, polarizability and classical theory of Raman spectrum. Rotational and vibrational Raman spectrum. Raman spectra of polyatomic molecules. Complementarity of IR and Raman spectra. Mutual exclusion principle. Introduction to instrumentation. Laser Raman spectrum.

Electronic spectra. Electronic spectra of diatomic molecules. Vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle. Types of electronic transitions. Fotrat diagram. Predissociation . Calculation of heat of dissociation.

Electronic spectra of polyatomic molecules: Electronic transition among molecular orbitals and absorption frequencies. Effect of conjugation. Introduction to instrumentation. Simultaneous determination of two components.

Unit III Irreversible thermodynamics 18 h

Thermodynamics of irreversible processes : Simple examples of irreversible processes. General theory of non equilibrium processes. Entropy production from heat flow. Matter flow and current flow. Generalised equation for entropy production. The phenomenological relations. Onsager reciprocal relation, Application of irreversible thermodynamics to diffusion. Thermal diffusion, Thermo osmosis and thermomolecular pressure difference., electro kinetic effects, the Glansdorf- Pregogin equation. Far from equilibrium region. Principle of minimum entropy production. Thermodynamic analysis of stability. Stability criterion and Le-Chatelier Brawn Principle.

Unit IV Statistical mechanics -I 18 h

Mechanical description of molecular systems. Thermodynamic probability and entropy. Microstates. Concept of ensembles Canonical and Grand canonical ensemble. Maxwell Boltzmann distribution.

Quantum statistics: Bose Einstein Statistics , Bose Einstein distribution. Thermodynamic probability, Bose Einstein distribution function. Examples of particles. Theory of Para magnetism. Bose Einstein condensation, Liquid Helium. Supercooled liquid. Fermi- Dirac Statistics. Fermi- Dirac Distribution, Examples of particles, Fermi Dirac Distribution function Thermionic emission. Relation between Maxwell Boltzmann, Bose Einstein and Fermi - Dirac Statistics The Partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration. Complex partition functions and partition function for particles in different force fields. Langevin‟s partition function and its use for the determination of dipole moment.

Unit V Electrochemistry 18 h

Ionics- Ions in solution. Deviation from ideal behaviour. Ionic activity. Ion-solvent interaction. Born equation. Ion-ion interaction. Activity coefficient and its determination. Debye-Huckel limiting law. Equation for appreciable concentration. Osmotic coefficient. Activities in concentrated solutions. Ion associations. Strong electrolytes. Ion transport. Debye-Huckel treatment. Onsager equation. Limitation of the model. Conductance at high frequencies and high potentials.

Electrodics: Different type of electrodes. Electrochemical cells. Concentration cells and activity coefficient determination. Origin of electrode potential. Liquid junction potential. Evaluation of thermodynamic properties. The electrode double layer. Electrode-electrode interface. Theory of multilayer capacity. Electrocapillarity. Lippmann potential and membrane potential.

Fuel cells- H_2-O_2 fuel cell, fuel cell for high temperature applications.

Electrokinetic phenomena. Mechanism of charge transfer at electrode- electrolyte interface. Electrolysis. Current- potential curve. Dissolution, deposition and decomposition potentials. Energy barriers at metal -electrolyte interface. Different types of overpotentials. ButlerVolmer equation. Tafel and Nernst equation. Rate determining step in electrode kinetics. The hydrogen and oxygen over voltage. Theories of overvoltage.

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SEMESTER III

15PCH 31 INORGANIC CHEMISTRY- III

Total 90 h

Unit I Organometallic compounds 18 h

Nomenclature of organometallic compounds.Types of metal complexes. Metal carbonyls, bonding in metal carbonyls. Application of infrared spectroscopy for the elucidation of metal carbonyl bonding. Bonding in metal nitrosyls and cyanides. Synthesis, structure and bonding in polynuclear carbonyls with and without bridging. Complexes with linear π- donor ligands: Olefins, acetylenes, dienes and allyl complexes. Hapto nomenclature. Complexes with cyclic π donors: Cyclopentadiene, benzene, cycloheptatriene and cyclooctatetraene complexes, structure and bonding. Fluxional molecules. Catalysis by organometallic compounds: Hydrogenation, hydroformylation and polymerization reactions.

Unit II Reactions of metal complexes 18 h

Energy profile of a reaction - Thermodynamic and kinetic stability, Classification of ligand substitution reactions -kinetics and mechanism of ligand substitution reactions in square planar complexes, trans effect- theory and synthetic applications.

Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic)

Electron transfer reactions: Outer sphere mechanism- Marcus theory, inner sphere mechanism- Taube mechanism. Photochemical reactions- substitution and redox reactions of Cr(III) , Ru(II) , and Ru(III) complexes. Photo-isomerisation and photo-aquation reactions of metal complexes.

Unit III Metal-metal bonds and metal clusters 18 h

Metal-metal bonds: Factors affecting the formation of metal-metal bond. Dinuclear compounds of Re , Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, Trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains. Metal carbonyl clusters. Anionic and hydrido clusters. LNCCs and HNCCs. Isoelectronic and isolobal relationships. Hetero atoms in metal clusters: Carbide and nitride containing clusters. Electron counting schemes for HNCCs. Capping rule. Chalcogenide clusters. Chevrel phases.

Unit IV Bioinorganic chemistry 18 h

Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium pump. Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis. Role of calcium in biological systems.

Oxygen carriers and oxygen transport proteins- haemoglobin, myoglobin and haemocyanin. Iron storage and transport in biological systems- ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes- CarboxypeptidaseA- structure and functions. Nitroeenaesesgeases, biological nitrogen fixation. Vitamin B_{12} and coenzymes.

Unit V Errors in Chemical Analysis **18 h**

Evaluation of analytical data: Accuracy and precision. Standard deviation, variance and coefficient of variation. Student t-test. Confidence limits. Estimation of detection limits. Errors: Classification, distribution, propagation, causes and minimization of errors. Significant figures and computation rules. Correlation analysis: Scatter diagram. Correlation coefficient (r). Calculation of r by the method of least squares. Systematic and random errors. Distribution of experimental results. Statistical treatment- standard deviation, variance, confidence limits, application of statistics to data treatment and evaluation, student-t and f tests, detection of gross errors, rejection of a result-Q test, estimation of detection limits.

Least square method, correlation coefficient and its determination. Hypothesis testing using statistical analysis. Using spread sheets for plotting calibration curves. Quality assurance and control charts.

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15PCH 32 ORGANIC CHEMISTRY-111

Total 90 h

Unit 1 Organic spectroscopy 18 h

Organic mass spectroscopy. EI, CI, FAB, Electrospray and MALDI ion sources. Magnetic, High resolution (Double focusing), TOF and quadruple mass analysers. Characteristic EIMS fragmentation modes and MS rearrangements. Mass spectral fragmentation patterns of long chain alkanes, alkenes, alkynes, carbonyl , nitro, amino and carboxy compounds. Strategies for the analysis of mass spectra.

Theory of NMR spectroscopy, chemical shifts, anisotropic effects and coupling constant. Spin-spin interactions in typical systems. First order and second order spectra. Simplification methods of complex spectra by high field NMR, shift reagents, chemical exchange and doule resonance. ^{13}C NMR chemical shifts. Applications of NOE, APT, DEPT, INEPT and 2D-NMR and INADEQUATE, HOHA spectroscopies. Introduction to 3D NMR.
Spectral interpretations and structure identification.

Unit II Molecular recognition and Supramolecular chemistry 18 h

Introduction to supramolecular chemistry. One-pot reactions.The concepts of molecular recognition, host, guest and receptor systems. Forces involved in molecular recognition. Hydrogen bonding, ionic bonding, π-stacking, Vander Walls and hydrophobic interactions. Introduction to molecular receptors. Tweezers, cryptands and carcerands. Cycophanes, cyclodextrins and calixarenes- typical examples. Non-covalent interactions in biopolymer structure organization. Role of self organization and self association in living nature.

Importance of molecular recognition in DNA and protein structure, their function and protein biosynthesis. Supramolecular systems like Organic zeolite, Clathrate hydrates of gases, Helicates. Nanotubes, liquid crystals, nanotechnology and other industrial applications of supramolecular chemistry.

Unit III Medicinal chemistry 18 h

Retrosynthetic analysis and disconnection approach. Synthetic strategy and synthons**,** Combinatorial organic synthesis, introduction, methodology, automation, solid supported and solution phase synthesis, study of targeted or focused libraries and small molecule libraries. Application- drug discovery. Drug design and development: Discovery of a drug, a lead compound, Development of drug-Pharmaccophore identification, modification of structure, structure-activity relationship, structure modification to increase potency. The Hammet equation,Taft equation and lipophilicity. Computer assisted drug design. Receptors and drug action. Natural products and drug development. Different classes of drugs with examples. Synthesis of paracetamol, phenobarbital, diazepam, sulphamethoxazole, benzyl penicillin, chloramphenicol.

Unit IV Green chemistry 18 h

Twelve principles of green chemistry. Green chemical strategies for sustainable development- Reaction mass balance, atom economy evaluation for chemical reaction efficiency, green solvents, reaction media- Synthesis under water, solventless, fluorous and ionic liquid media. Synthesis using scavenger resins, catalysis and biocatalysis. Green computation. Green processes-. Microwave synthesis**-** fundamentals of microwave synthesisTwo Principal Mechanisms for Interaction With Matter- The Microwave Effect with examples - Single-Mode and Multimode Microwave cavities. Microwave technologyTechniques and applications in MORE chemistry. Sonochemical synthesis. Applications of sonication in the synthests of organic compounds.

Unit V Chemistry of biopolymers and polymers 18 h

Peptide bond formation methods. Amino and carboxy protection in SPPS. Synthesis of A, G,C, T, U adenosine, ADP and ATP. Automated polypeptide and oligonucleotide synthesis. Structure organization of proteins and poly nucleotides. Protein sequencing by Edmans method. Protein denaturation. Structure of polysaccharides including starch, cellulose,glycogen and chitin. Classes of polymers-Types and mechanisms of polymerization reactions. Methods of molecular mass and size distribution determination. Polymer structure and property characterization. Synthesis of stereo regularpolymers. Ziegler-Nattacatalyst.Polymers in organic synthesis- supports, reagents and catalysts. Bio degradable polymers.

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15PCH 33 Physical Chemistry -III

Total 90 h

Unit I Computational chemistry. 18 h

Introduction to computational chemistry, concept of potential energy surface(PES), stationary point, saddle point and geometry optimisation.

Basis sets, STO, Gaussian functions and its properties, GTO, contracted Gaussians, minimal , split valance, polarised and diffused basis sets.

Introduction to SCF. Wave function for open shell state, RHF, ROHF and URHF. Model

Chemistry. Brief description of computational methods- ab-initio, semiempirical and density functional and molecular mechanics methods. Construction of Z-matrix for simple molecules- H_2O, H_2O_2, H_2CO, CH_3CHO, NH_3, and CO_2.

Unit II Spectroscopy II 18 h

Resonance spectroscopy: Nuclear Magnetic resonance Spectroscopy, Nuclear spin. Interaction between nuclear spin and applied magnetic field. Proton NMR . Population of energy levels. Nuclear resonance. Chemical shift. Relaxation methods. Spin-spin coupling. Fine structure. Elementary idea of 2D and 3D NMR. Introduction to instrumentation.

ESR spectroscopy: Electron spin. Interaction with magnetic field. Kramer‟s rule. The g factor. Determination of g values. Fine structure and hyperfine structure. Elementary idea of ENDOR and ELDOR.

Mossbauer spectroscopy: Basic principles. Doppler effect, chemical shift, recording of spectrum, application. Quadrupole effect. Principle and application of NQR spectroscopy.

Photoelectron spectroscopy. Introduction to UV photoelectron and X-ray photoelectron spectroscopy.

Unit III Surface chemistry 18 h

Different types of surfaces. Properties of surface phase. Thermodynamics of surface. Surface tension of solutions. Gibb’s adsorption equation and its verification. Surfactants and miscelles.

Surface films: different types, Surface pressure and Surface potential, and their measurements and interpretation.

The Gas- solid inter phase. Types of adsorption. Heat of adsorption, The Langmuir theory kinetic and statistical derivation. Multilayer adsorption- the BET theory and Harkins- Jura theory. Adsorption from solutions on solids. Langmuir and classical isotherms. Chemisorption-. differences with physical adsorption. Adsorption isotherms, adsorption with dissociation. Adsorption with interaction between adsorbate molecules.

Measurement of surface area of solids: Harkins - Jura absolute method, entropy method and the point B method. Use of Langmuir, BET and Harkins - Jura isotherms for surface area determination.

Dispersed systems: Types of dispersions; Spontaneous self-organization; Surfactants: structure of surfactants in solution; critical micellation concentration (CMC); temperature dependence; influence of chain length and salt concentration; surfactant parameter. Emulsions: macro- and micro-emulsions; aging and stabilization of emulsions; Phase behaviour of microemulsions. Colloids, vesicles, lipid bilayer membrane

Unit IV Industrial Catalysis

Introduction, specific and general catalysis, prototropic and protolytic mechanism with examples, acidity function the importance of catalysis in industry and society and basic principles, physical adsorption and chemisorption on surfaces, adsorption isotherms. Adsorption and heterogeneous catalysis, rate models: Langmuir-Hinshelwood and Mars Van Krevelin, bonding of reactants to catalyst surfaces, specific surface areas and porosity, pore size distribution, Kinetics for catalytic reactions, Adsorption – kinetics. catalyst preparation, evaluation of catalytic activity, catalytic reactor types and conditions of use., Structured catalysts and zeolite, Catalyst characterization by SEM, XRD, gas adsorption and other techniques Catalyst deactivation, Acid catalysis and zeolites, Processing of petroleum and hydrocarbons. Catalytic oxidation. Synthesis gas and associated processes. Steam reforming. The water gas shift reaction. Methanation. Ammonia production. Nitric acid. Methanol and formaldehyde. Fischer-Tropsch. Catalysis for environmental protection and energy production. The fuel cell for vehicles, Catalytic processes for bio-ethanol production, Catalytic processes for biodiesel production, Biomass conversion to fuels, Three Way catalytic converters for automobiles. Oxygen sensors, Deactivation, Control of diesel emissions.

Unit V Electro Analytical methods. 18 h

Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Chemfets-importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations-types and applications. 1.2 Polarography and voltametric techniques: micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography

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15PCH 34 Inorganic Chemistry Practicals -II Total-125 h

1. Estimation of simple mixture of ions (involving quantitative separation) by volumetric and Gravimetric methods.

2. Analysis of typical alloys and ores

3. Ion exchange separation of binary mixtures.

4. Spectral Interpretation of metal complexes using IR, UV-Vis. spectral data. Supplementary information like metal estimation, CHN analysis, conductivity measurements and magnetic measurements to be provided to the students. Assessment is based on arriving at the structure of the complex and assignment of IR spectral bands.

5. Interpretation of TG and DTA curves of metal oxalates/acetates/sulphates/chlorides in hydrated forms. Assessment is based on the identification of various stages.

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9. E. A. O. Ebsworth, „Structural methods in chemistry‟ Blackwell Scientific Publications.

15PCH 35 ORGANIC PRACTICALS-II

Total 125 h

A.Volumetric estimation of

1) Aniline 2) Phenol 3) glucose

4) Iodine value and saponification value of coconut oil

B). **Colorimetric estimation** of 1) Aniline 2) Glucose 3) Cholesterol 4) Ascorbic acid 5) Streptomycin or Aspirin.

C). Spectral identification (UV, IR, ^{1}H NMR, ^{13}C NMR, EI mass) of Organic compounds from a library of organic compounds

D. Separations of mixtures by Paper Chromatography

1) Separation of amino acids 2) Separation of dyes

E) Three stage preparation

1)Benzaldehyd**e to** Benzoin(green synthesis with thiamine HCl) **to** benzyl benzilic acid

2) Phthalic acid **to** Phthalic anhydride **to** pthalimide anthranilic acid

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15PCH 36 PHYSICAL PRACTICALS -II Total 125 h

1. Conductometry

Determination of strength of strong and weak acids in a mixture Determination of strength of a weak acid.

Determination of solubility product of a sparingly soluble salt ($PbSO_4$, $BaSO_4$ etc.) Hydrolysis of NH_4Cl or CH_3COONa or aniline hydrochloride

Determination of order of reaction, rate constant and energy of activation for saponification of ethyl acetate

Precipitation titrations.

Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from measurement of conductivities at different concentrations.

Equivalent conductance at infinite dilutions and verification of Kohlraush‟s Law. Determination of Onsager constants.

2. Potentiometry

Determination of emf of Daniel cell.

Determination of the emf of various $ZnSO_4$ solutions and hence the concentration of unknown $ZnSO_4$ solution.

Determination of valency of mercurous ion.

Determination of temperature dependence of EMF of a cell

Determination of stoichiometry and formation constant of silver-ammonia complex. Determination of activity and activity constant of electrolytes. Determination of thermodynamic constants of reactions. pH metric titrations.

Acid alkali titrations using Quinhydrone electrode.

Titrations(double) involving redox reactions - Fe^{2+} Vs $KMnO_4$, $K_2Cr_2O_7$, $Ce(NH_3)SO_4$ and KI Vs $KMnO_4$

Determination of strengths of halides in a mixture.

Determination of pH of buffer solutions and hence to calculate the E_0 of quinhydrone electrode

3. Spectrophotometry

Verification of Beer-Lambert‟s law.

Absorption spectra of conjugated dyes.

Determination of concentration of potassium dichromate and potassium permanganate in a mixture.

To study the complex formation between Fe^{3+} and salicylic acid.

Determination of pKa of an indicator.

4. Polarimetry

Measurement specific rotation of glucose.

Determination of specific rotation of sucrose

Determination of unknown concentration of glucose solution.

and rate constant of its hydrolysis in presence of HCl

5. Polarography :

Determination of half wave potential E ½ and unknown concentration of Cd^{2+} ion.

Determination of concentrations of metal ions in a mixture.

6. Surface tension

Determination of surface tension of various liquids by Stalagmometric method (drop number / drop weight)

Determination of parchors of molecules and various groups.

Determination of concentration of a mixture.

Determination of surface tension and parachor of liquids using double capillary method.

7. Refractometry

Determination of molar refraction of pure liquids

Determination of concentration of KCl solution/glycerol solution

Determination of solubility of KCl in water.

Determination of molar refraction of solid KCl

Study the stoichiometry of potassium iodide-mercuric iodide complex.
Determination of concentration of KI solution.

8. Viscosity

Determination of viscosity of various liquids using Ostwald,s viscometer.

Determination of unknown composition of given liquid mixture like toluene-nitrobenzene.

Verification of Kendall‟s relation.

Verification of Jon Dole‟s equation.

References

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J. M. Newcombe, R. J. Denaro, A. R.Rickett, R.M.W Wilson,"Experiments in Physical

Chemistry"Pergamon.

A.M.James, and F.E.Pichard, "Practical Physical Chemistry", Longman.

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B.Viswanathan, „"Practical Physical Chemistry", Viva Publications.

P.S.Sindhu, "Practicals in Physical Chemistry-A Modern Approach", MacMillan India.

D. P. Shoemaker, C. W. Garland & J. W. Nibler. "Experiments in Physical Chemistry", McGraw Hill.

SEMESTER IV

15PCH 41 (a) ADVANCED INORGANIC CHEMISTRY

Total 90 h

Unit I Spectroscopic methods in inorganic chemistry-I 18 h

Infrared and Raman spectroscopy: Vibrational modes, group frequencies of infrared systems, factors affecting the group frequencies, study of hydrogen bonding effects, infrared spectra of coordination compounds. Structural elucidation of coordination compounds containing the following molecules/ ions as ligands- NH_3, H_2O, CO, NO, OH^- , SO_4^{2-} , CN^- , SCN^- , NO_3^- NO_2^- CH_3COO^- and X^- (X= halogen).

Changes in ligand vibration on coordination with metal ions. Vibrational spectra of metal carbonyls- CD and ORD spectra of metal complexes.

Physical characterization of inorganic compounds by UV, NQR and MS techniques.

Unit II Applications of group theory 18 h

Hybrid orbitals and molecular orbitals for simple molecules. Transformation properties of atomic orbitals. Hybridastion schemes for σ and π bonding with examples. MO theory for AB_n type molecules. Molecular orbitals for regular octahedral, tetrahedral and metal sandwich compounds.

Ligand field theory: Splitting of d orbitals in different environments using group theoretical considerations. Construction of energy level diagrams. Correlation diagram. Method of descending symmetry. Tanabe-Sugano diagrams. Selection rules for electronic spectra. Molecular orbitals in octahedral complexes. Formation of symmetry adapted group orbitals of ligands. MO diagram.

Symmetry and selection rules: Symmetry properties of common orbitals. Application of character tables to infrared and Raman spectroscopy. Infrared and Raman active modes for C_{2v}, C_{3v} and D_{4h}

Unit III Spectroscopic methods in Inorganic chemistry -II 18 h

ESR spectra of metal complexes: Hyperfine splitting and A parameter, g values, zero field splitting and Kramers degeneracy. Application to Cu(II) complexes and inorganic free radicals such as PH_4, F_{2-} and $[BH_3]^-$.

Nuclear Magnetic Resonance Spectroscopy :The contact and pseudocontact shifts, factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides with emphasis on ^{31}P and ^{19}F NMR.

Mossbauer Spectroscopy : Basic Principles, spectral parameters and spectrum display. Application of the technique to the studies of iron and tin complexes.

Unit IV Introduction to molecular clusters

Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the closo-, nido-, arachno-borane structural paradigm, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.

Transition-metal clusters: Low nuclearity metal-carbonyl clusters and 14n+2 rule, high nuclearity metal-carbonyl clusters with internal atoms. Structure, synthesis and reactivity. Capping rules, isolobal relationships between main-group and transition metal fragments, metal-ligand complexes vs heteronuclear cluster.

Main-group-Transition-metal clusters: Isolobal analogs of p-block and d-block clusters, limitations and exceptions.

Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters.

Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides.

Illustrative examples from recent literature.

Unit V Bioinorganic chemistry and Inorganic medicinal chemistry 18 h

Copper on biochemical systems. Oxidase activity, super oxide dismutase activity. Electron transport in biology. Structure and function of copper proteins in electron transport process. Oxygen transport copper proteins. Hemocyanin- copper transport, copper enzymesAzurin, plastocyanin.

Inorganic medicinal chemistry. Metals in medicine. Metal toxicity and homeostasis. Metal deficiency and diseases. Toxic effects of metals. Effect of deficiency and excess of essential metal ions. Toxicity due to non essential elements and speciation. Detoxification mechanism. Role of lithium and aluminium in biological systems. Chelation therapy and chemotherapy. Anticancer drugs and vanadium based diabetic drugs.

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4. F. A. Cotton and G. Wilkinson, „Advanced Inorganic Chemistry‟, John Wiley and Sons.
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21. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, „Bioinorganic chemistry"

15PCH 41 (b) - ADVANCED ORGANIC CHEMISTRY

Unit I Reagents in organic synthesis 18 h

Applications of hydrogenation catalysts, hindered boranes, bulky metal hydrides. $NaCNBH_3$, DIBAL, Li trialkylborohydrides, tri-n-butyl tin hydride, diimide, Lindlar catalysts and aluminium alkoxide. Rosenmund reduction and McFadeyan-Stevens reaction. Oxidation using SeO2, lead tetraacetate, ozone, peracids, DDQ, manganese 1V oxide, silver carbonate and

Cr(V1) reagents. Swern oxidation, Moffatt oxidation, allylic and benzylic oxidation. Sommelet reaction. Elbs reaction. Oxidative coupling of phenols. Sharpless asymmetric epoxidation. Chemo and regioselectivity in reductions and oxidations. Use of XeF_2, SbF_5, VF_5, MoF_6, CF_3OF, SF_4, HF and F_2as fluorinating agents.

Unit II Organomatallic chemistry 18 h

Preparation of organo Mg, Al, Li, Cu, Zn, Cr, Fe, Ce and sulphur stabilised compounds. Reactions of Grignard reagents in organic synthesis. Alkylation, oxirane addition, carbondioxide addition, carbonyl addition, enone addition (1,2 and 1,4additions), reduction, conjugate addition and enolisation reactions. Selectivity in Grignard reactions. Reactions of organo Li reagents, Li exchange reaction, its use in the preparation of RLi compounds, addition to C=O, COOH and $CONR_2$, Li dialkyl cuprates (Gilman reagent)-preparation and reaction with alkyl halides, aryl halides, with enones. Alkynyl Cu(1) reagents, Glaser coupling. Dialkyl Cd compounds- preparation and reaction with acyl halides. Benzenetricarbonyl chromium- preparation and reaction with carbanions. Tebe reagent, Silane carbanion and its reactions.

Unit III Organic synthesis 18 h

C-C and C=C bond forming reactions. Mannich, Riemer-Tiemann, Simon-Smith, VilsmeierHack, Ullmann and Chichibabin reactions. Ring formation by Dieckmann, Kostanecki, Thorpe, Pschorr and acyloin condensations. Stork enamine, Shapiro, Peterson, Heck, Stille, Ritter and Prilezhaev reactions. Synthesis of small rings. Simon-Smith reaction. Reduction and oxidation in synthesis. Catalytic hydrogenation. Alkali metal reduction, Birch reduction, Wolff-Kishner reduction and Clemmenson reduction. Huang-Milon modification. Boranes, LAH and sodiumborohydride as reductants. Hydrogenations, Oppenauer oxidation, Jones oxidation. Applications of HIO_4, OsO_4 and mCPBA.

Unit IV Methods in organic synthesis 18 h

Sterospecific and steroselective synthesis, Sharpless asymmetric epoxidation, Chiral pool, chiral auxiliary, Chiral reagents, BINAP, Regioselectivity in enol and enamine alkylation.

Stereoselective and stereospecific synthesis. Mitsunobu reaction. 1,3-dipolar cycloaddition in the construction of rings. Story synthesis. Olefin synthesis by extrusion reactions. Olefin metathesis. Umpolung. Reductive coupling reactions. Epoxide to alkene. Introduction to combinatorial synthesis. Electrochemical reduction of organic halogen, nitro and carbonyl compounds. Electrochemical Kolbe oxidation. Tetrahydropyranyl, silyl, t-butyl, trichloroethyl, acetal and thioacetal as hydroxyl, thiol, carboxyl and carbonyl protecting groups in synthesis.

Unit V Construction of Carbocyclic and Heterocyclic Ring Systems and Protecting Group Chemistry

18 h

Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered ringsoxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization. 3.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis. 35 3.3 Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection. Illustration of protection and deprotection in synthesis. 4.2 Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups used in solution phase and solid phase peptide synthesis (SPPS). 4.3 Functional equivalence and reactivity Umpolung. Role of trimethyl silyl group in organic synthesis.

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SEMESTER IV

15PCH 41(c) ADVANCED PHYSICAL CHEMISTRY

Total 90 h

Unit I Applications of group theory 18 h

Spectroscopic applications: Transition moment integral transition moment operator. Vanishing matrix element. Symmetry selection rule for IR, Raman and electronic spectra. Dipole and polarizability transition moment operator. Identification of IR and Raman active normal modes in molecules coming under various point groups such as C_{2v}, C_{3v}, C_{4v}, D_{3h}, T_d and O_h. Mutual exclusion and complementarity principle of IR and Raman spectra and their use in the identification of molecular structures. Probability of overtone and combination bands. Identification of allowed and forbidden electronic transitions in carbonyl groups. Vibronic transitions.

Application to MO theory: Symmetry adapted LCAO-MO theory of π-bonded hydrocarbons. Projection operator and its use in the construction of wave functions of π-molecular orbitals, secular equations and use of symmetry for simplifying the calculations of energy and wave functions of ethylene, butadiene and carbocyclic systems such as benzene and naphthalene.

Unit II Exactly solvable systems. 18 h

Simple Harmonic Oscillator: Wave equation for ID harmonic oscillator. Complete solution and their properties. Three dimensional Harmonic oscillator. Potential energy in three dimension and Schrodinger wave equation in Cartesian coordinate. Separation of variables and solution of the equation for energy and wave function. Degeneracy.

Rigid rotor: Schrodinger equation in polar Coordinate. Angular momentum operator for rigid rotor. Separation of variables and complete solution for phi and theta equations. Legendre polynomials and associated Legendre functions. Normalisation of associated Legendre functions and evolution of the values of orbital angular momentum quantum number. Recursion relations. Rigid rotor wave function and energy.

The Hydrogen atom: Schrodinger wave equation in polar coordinate. Separation of variables and complete solution of the radial part. The associated Laguarre polynomial. Normalisation. The evolution of the value of the principal quantum number. The spherical harmonics and the radial part of the wave function. The total wave function of H atom. The wave functions of Hydrogen like atomic orbitals and explanations for the shapes of various orbitals.

Angular momentum, angular momentum operators(L_x,L_y,L_z and L^2) and their commutation properties. Spherical harmonics as eigen functions of angular momentum operator L_z and L^2. Ladder operator method for angular momentum. Space quantisation.

Unit III Approximate method I 18 h

Schrodinger wave equation for He atom and anharmonic oscillator and difficulty to get the exact solution. The Variation method: Variation theorem and its proof. The variation integral and its properties. Variational parameters. Trial wave functions, Illustration of trial wave functions for calculation of H atom and particle in a 1D box as examples.

Trial functions as linear combination of orthonormal functions, linear combinations of functions containing variational parameters as trial functions. Setting up of secular determinants. Variation methods of normal state of He . The SCF method, SCF and variation method. Strength and limitation of the method.

Unit IV Approximate method II 18 h

The perturbation method. The generalised perturbation method. The idea of successive correction to unperturbed systems. First order perturbation. Correction of wave function and energy . Theory of non-degenerate level perturbation.The normal Helium atom. The first order perturbation of the degenerate level. The hydrogen atom. Second order perturbation theory. Correction for wave function and energy. Stark effect. Time dependant wave equation: Variation in the state of a system with time. Emission and absorption of radiation. The Einstein‟s transition probability and its calculation. Selection rules and intensity of spectrum for harmonic oscillator , rigid rotor and hydrogen atom.

Unit V Computational methods 18 h

Computational methods as potential tools for practicing chemistry. Potential energy surface, saddle point, local minima and global minima. Geometry optimisation. Exchange and overlap integrals. Difficulty in evaluating them with H-like wave functions. Slater Type functions(STO), approximation of STO with Gaussian type functions. Contracted Gaussians.

Basis sets: minimal basis set, split valance basis set, polarised basis set and diffused basis set. Model chemistry and notations.

Geometry input- in terms of Cartesian coordinates and internal coordinates. Z-matrix, construction of z-matrices of simple molecules H_2, H_2O, H_2O_2, H_2CO,CH_3CHO, CH_4, C_2H_6 and with dummy atom, CO_2, NH_3,C_6H_6.

Molecular mechanics method: Force fields, potential energy expressions for bond stretching, bending, torsion, non-bonded interactions, electrostatic interaction and H-bonding. Setting up of force field expressions. Method of parameterisation. Use of molecular mechanics. Brief introduction to commonly using force fields(MM3, MMFF, AMBER and CHARMM) and Softwares.

Ab-initio method: Hartree-Fock Self Consistent Field method. Slater determinant. Post Hartree-Fock methods- Configuration Interaction(CI) and Moller Plesset(MP)methods.

Semiempirical method: Basic principle of the method. Its variants, ZDO,CNDO and INDO. Density Functional method: Functional. Hohenberg-Kohn theorems. Kohn-Sham orbitals. Basic idea of Local Density(LD) approximation, Generalised Gradient approximation and hybrid (BLYP, B3LYP) methods.

Comparative study of Molecular Mechanics, Ab-initio method, Semi-empirical method and DFT method of computations.

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12 E. Lewars, “Computational Chemistry- Introduction to the Theory and Applications of Molecular and Quantum Mechanics”, Springer.

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15PCH 42 (a) DISSERTATION

Each of the students has to carry out original research in a topic in accordance with the Elective paper chosen for Semester IV under the guidance and supervision of a teacher in the concerned Department of the College.

Instructions to Question Papers Setters

The Syllabus of each theory has five units. While setting the question papers, equal weight is to be given to each of the Units for choosing the questions. Each question paper is of 3 hours duration and has three Sections, namely Section A, Section B and Section C constituting a total 75 marks as detailed.

Section A- Five questions, one from each Unit containing three short answer questions marked (a), (b), and (c), each of which has 2 marks. One has to answer any two of (a), (b) or (c) from each of the five questions. (2x10 = 20 marks)

Section B- Five questions, one from each Unit containing two short essay questions marked (a) and (b), each of which has **4** marks. One has to answer either (a) or (b) from each of the five questions. (4x5 = 20 marks)

Section C- Five essay questions, one from each unit having 10 marks. One has to answer any three questions from the five questions asked. (10x3 = 30 marks)