

Course Structure & Syllabus
for
M.Sc. Physical Chemistry

(Syllabus for Semesters I & II is common for M.Sc. Analytical Chemistry and

M.Sc Organic Chemistry and M.Sc Physical Chemistry)

2019-2020



ADIKAVI NANNAYA UNIVERSITY

Rajamahendravaram

Course structure for Physical Chemistry.docx

FIRST SEMESTER(2019-20).docx

SECOND SEMESTER(2019-20).docx

Course Structure of M.Sc. Physical Chemistry

S. No.	Semester	Code of the paper	Title of the paper	Theory/ Practical /Viva	Internal marks	External marks	Total marks	Credits
1.	Semester-I		General Chemistry-I	T	25	75	100	4
2.			Inorganic Chemistry-I	T	25	75	100	4
3.			Organic Chemistry-I	T	25	75	100	4
4.			Physical Chemistry-I	T	25	75	100	4
5.			Inorganic Chemistry Practical-I	P	25	75	100	3
6.			Organic Chemistry Practical-I	P	25	75	100	3
7.			Physical Chemistry Practical-I	P	25	75	100	3
8.	Semester-II		General Chemistry-II	T	25	75	100	4
9.			Inorganic Chemistry-II	T	25	75	100	4
10.			Organic Chemistry-II	T	25	75	100	4
11.			Physical Chemistry-II	T	25	75	100	4
12.			Inorganic Chemistry Practical-II	P	25	75	100	3
13.			Organic Chemistry Practical-II	P	25	75	100	3
14.			Physical Chemistry Practical-II	P	25	75	100	3
15.	Semester-III		Advanced Chemical Kinetics and Physical Chemistry of Polymers	T	25	75	100	4
16.			Quantum Chemistry and Chemical applications of Symmetry and Group theory	T	25	75	100	4
17.			Statistical Thermodynamics and Solution equilibria of proton ligand complexes	T	25	75	100	4
18.			Instrumentation	T	25	75	100	4
19.			Kinetics-I	P	25	75	100	4
20.			Instrumentation-I	P	25	75	100	4
21.	Semester-IV		Advanced Chemical kinetics and photochemistry	T	25	75	100	4
22.			Quantum Chemistry and numerical methods for chemists and advanced computer programming	T	25	75	100	4
23.			Advanced thermodynamics and solution equilibria of metal ligand complexes	T	25	75	100	4
24.			Spectroscopy	T	25	75	100	4
25.			Kinetics-II	P	25	75	100	4
26.			Instrumentation-II	P	25	75	100	4
27.				Comprehensive viva-voce	V	----	50	50
					Total Credits			100

Note: I & II Semesters syllabus and course structure are common for M. Sc. Organic Chemistry/Analytical Chemistry /Physical Chemistry courses.



ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
FIRST SEMESTER- SYLLABUS
(With effect from 2019-20 admitted batch)

Paper- I: GENERAL CHEMISTRY-I

UNIT-1

Basic Quantum Chemistry-I Wave equation-interpretation of wave function-properties of wave function-normalization and orthogonalisation, Operators- linear and non-linear- commutators of operators. Postulates of quantum mechanics; setting up of operators to observables; Hermitian operator- Eigen values and Eigen functions of Hermitian operator; Expansion theorems. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

UNIT-II

Basic Quantum Chemistry-II Wave mechanics of simple systems with constant potential energy, particle in one-dimensional box- factors influencing color transition- dipole integral, Symmetry arguments in deriving the selection rules, the concept of tunneling- particle in three -dimensional box. Calculations using wave functions of the particle in a box- Orthogonality, measurability of energy, position and momentum, average values and probabilities. Rigid rotor, Wave mechanics of systems with variable potential energy-simple harmonic oscillator- solution of wave equation- selection rules.

UNIT-III

Fundamentals of Molecular Spectroscopy-I: Microwave and IR- Spectroscopy- Rotational spectra of diatomic molecules- Rigid rotor-Selection rules- Calculations of bond length- Isotopic effect, Second order stark effect and its applications. Infrared spectra of diatomic molecules- harmonic and anharmonic oscillators- Selection rules- Overtones- Combination bands- Calculation of force constant, anharmonicity constant and zero point energy. Fermi resonance, simultaneous vibrational-rotational spectra of diatomic molecules.

UNIT- IV

Fundamentals of Molecular Spectroscopy-II: Raman and Electronic Spectra- Classical and quantum mechanical explanations- Rotational Raman and Vibrational Raman spectra. Electronic spectra of diatomic molecules- Vibrational Coarse structure- intensities of spectral lines- Franck-Condon principle- applications, Rotational Fine structure- band head and band shading. Charge transfer spectra

References/ Text books

1. Fundamentals of Molecular spectroscopy: by C.N. Banwell
2. Molecular spectroscopy: by B.K.Sharma
3. Molecular spectroscopy: by Aruldas
4. Introductory quantum mechanics: by A.K. Chandra
5. Quantum chemistry: by R.K. Prasad



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Paper- II: INORGANIC CHEMISTRY-I

UNIT-1

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in π -bonding. Application of MO theory to Tetrahedral $[\text{CoCl}_4]^{2-}$, Square planar $[\text{PtCl}_4]^{2-}$ and Octahedral complexes $[\text{CoF}_6]^{3-}$, $[\text{Co}(\text{NH}_3)_6]^{3+}$. Classification of ligands based on π -bonding using MO theory. Walsh diagram for H_2O molecule.

UNIT-II

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes. Electron counting in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Heterocyclic inorganic ring systems: Boron–Nitrogen ($\text{H}_3\text{B}_3\text{N}_3\text{H}_3$), Phosphorus–Nitrogen ($\text{N}_3\text{P}_3\text{Cl}_6$) and Sulphur-Nitrogen (S_4N_4 , $(\text{SN})_x$) cyclic compounds.

Cage Compounds: Phosphorous oxides and Phosphorous sulphides.

Isopoly and heteropoly anions.

UNIT-III

Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series – Jahn – Teller effect, nephelauxetic effect – ligand field theory.

Term symbols – Russell – Sanders coupling – derivation of term symbols for various configurations. Spectroscopic ground states.

UNIT- IV

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

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

Reference books & Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999).
5. Inorganic Chemistry 5th Edition by Gary L. Miessler et al, Pearson Publications.



ADIKAVI NANNAYA UNIVERSITY
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Paper –III: ORGANIC CHEMISTRY -I

UNIT – I

Nature of bonding in organic molecules and Aromaticity

15 Hrs

(A) *Electronic Effects and Reactive intermediates*:- Inductive effect, Mesomeric effect (Resonance), Hyperconjugation, Steric effect, Tautomerism, Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes

(B) *Criteria of Aromaticity*:- Huckle's rule and MO Theory, aromaticity in benzenoid non-benzenoid compounds, Aromaticity in Charged and Fused-Ring Systems, Hetero-aromatic Systems, Annulenes: Cyclobutadiene, Benzene, 1,3,5,7-Cyclooctatetraene, [10] Annulenes- [12], [14], [16] and [18] annulenes, azulenes, fulvenes, fullerenes, ferrocene, anti-aromaticity and homo-aromaticity.

UNIT – II

Stereo Chemistry & Molecular representation of organic molecules

20 Hrs

(A) *Molecular Symmetry and Chirality*:- Symmetry elements, Definition and classification of Stereoisomers, Enantiomer, Diastereomer, Homomer, Epimer, Anomer, Configuration and Conformation, Configurational nomenclature: D,L and R, S nomenclature, Molecules with a single chiral center: Molecules with two or more chiral centers.

(B) *Geometrical Isomerism and Conformations of Cyclic Systems*:- Cis-trans, E, Z- and Syn & anti nomenclature, Methods of determining configuration of Geometrical isomers using physical, spectral and chemical methods, Stability, Cis-trans inter conversion. Conformations of cyclobutane, cyclopentane, cyclohexane, mono and disubstituted cyclohexanes.

(C) *Prochirality and Prostereoisomerism*:- Homotopic ligands and faces; enantiotopic ligands and faces; diastereotopic ligands and faces; nomenclature of enantiotopic ligands and faces (Pro-R, Pro-S, Re, Si carbonyl compounds and Alkenes)

(D) *Stereoisomerism in molecules without chiral Center* -Axial chirality Allenes, Alkylidene cycloalkanes, spiranes, nomenclature. *Atropisomerism*: Biphenyl derivatives, nomenclature. *Planar chirality*: Ansa compounds, paracyclophanes, trans-cyclooctene and Helicity.

UNIT – III

Heterocyclic compounds

15 Hrs

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. Chemistry of heterocyclic compounds, synthesis and reactivity of the following systems: Quinoline, Isoquinoline, Indole, Pyrazole, Imidazole, Oxazole, Isoxazole, Pyridazine, pyrimidine and Pyrazine.

UNIT - IV

Chemistry of some typical natural products (Alkaloids and Terpenoids)

10 Hrs

A study of the following compounds involving their isolation, structure elucidation, synthesis and biogenesis of *Alkaloids*; Atropine, Nicotine, and Quinine.

Terpenoids: α - Terpeneol, α -Pinene and Camphor.



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Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons).
2. Organic Chemistry, Paula Yurkanis Bruice, 4th Ed. (Printice Hall)
3. Organic chemistry-Clayden J. (Oxford)
4. Organic Chemsitry, Wade, L.G. Jr. 5th Ed. (Pearson)
5. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
6. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
7. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman).
8. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International).
9. Organic Chemistry, R. T. Morrison and R. N. Boyd (Prentice-Hall)
10. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
11. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International).
12. Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)
13. Heterocyclic Chemistry, J.A.Joule, K. Kills and G. F. Smith, Chapman and Hall
14. Heterocyclic Chemistry, T.L.Gilchrist, Longman Scientific Technical
15. Heterocyclic Chemistry, Raj.K. Bansal.
16. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.

REFERENCE BOOKS:

1. Chemistry of Natural Products, K.W.Bentley
2. Stereochemistry of carbon compounds by E.Eliel, John Wiley & Sons, Inc.
3. Stereochemistry to Organic Compounds, D. Nasipuri, 2nd Ed. (New Age International).
4. Chemistry of Natural products by R.S. Kalsi Kalyani Publishers. 1983.



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Paper – IV: PHYSICAL CHEMISTRY-I

UNIT-I:

Thermodynamics-I: Concepts of partial molar properties – partial molar volume and its significance; Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Partial molar free energy, chemical potential, Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance. Phase equilibrium- Derivation of phase rule from the concept of chemical potential. *Ideal solutions* - Thermodynamic properties of ideal solutions mixing quantities; Vapour pressure-Raoult's law; Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Non-ideal systems -Concept of fugacity, fugacity coefficient. Determination of fugacity; Non ideal solutions. Activities and activity coefficients; Standard-state conventions for non ideal solutions; Determination of activity coefficients from vapour pressure measurements. Activity coefficients of non-volatile solutes using Gibbs-Duhem equation. Chemical equilibrium-effect of temperature on equilibrium constant- Van'tHoff equation

UNIT-II:

Micelles and Macro molecules: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization- phase separation and mass action models, Solubilization, micro emulsion, reverse micelles.

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of free radical polymerization. Molecular mass- Number and mass average molecular weight, molecular weight determination-End group analysis, Osmometry, viscometry, ultracentrifugation and light scattering methods.

UNIT-III:

Chemical Kinetics: Theories of reaction rates- Collision theory- Limitations, Transition state theory. Effect of ionic strength - Debye Huckel theory-Primary and secondary salt effects; Effect of dielectric constant, effect of substituent, Hammett equation-limitations, Taft equation; Prediction of rate constants- Consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation). Specific and general acid-base catalysis; Skrabal diagram; Fast reactions- different methods of studying fast reactions- flow methods, relaxation methods- temperature jump and pressure jump methods.

UNIT-IV:

Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules- singlet and triplet states, spin-orbit interaction. Quantum yield and its determination; Actinometry - ferrioxalate and uranyl oxalate actinometers-problems. Derivation of fluorescence and phosphorescence quantum yields. Quenching effect- Stern Volmer equation. Photochemical equilibrium and delayed fluorescence - E type and P type. Photochemical primary processes, types of photochemical reactions-photodissociation, addition and isomerisation reactions with examples.



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Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
3. Physical Chemistry by W.J.Moore, Prentice Hall
4. Thermodynamics for Chemists, Samuel Glasstone
5. Chemical Kinetics by K.J.Laidler, McGraw Hill Pub.
6. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
7. Polymer Chemistry by Billmayer
8. Introduction to Polymer Science, V.R. Gowriker, N.V.Viswanadhan and J. Sreedhar., Wiley Easter.
9. Micells, Theoretical and applied aspects, V.Morol, Plenum publishers.



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LABORATORY WORK (6 hrs/week)

Practical-1

INORGANIC CHEMISTRY PRACTICALS - I

I. Inorganic Synthesis: Preparation of

- (i) Tetraamminecopper(II) sulphate
- (ii) Potassium tris(oxalato)ferrate(III) trihydrate
- (iii) Tris(thiourea)copper(I) sulphate

II. Semi micro qualitative analysis of six radical mixtures

(One interfering anion and one less familiar cation for each mixture)

Anions: CO_3^{2-} , S^{2-} , SO_3^{2-} , Cl^- , Br^- , I^- , NO_3^- , SO_4^{2-} , CH_3COO^-
 $\text{C}_2\text{O}_4^{2-}$, $\text{C}_4\text{H}_4\text{O}_6^{2-}$, PO_4^{3-} , CrO_4^{2-} , AsO_4^{3-} , F^- , BO_3^{3-}

Cations: Ammonium (NH_4^+)
1st group: Hg, Ag, Pb, Tl, W
2nd group: Hg, Pb, Bi, Cu, Cd, As, Sb, Sn, Mo
3rd group: Fe, Al, Cr, Ce, Th, Ti, Zr, V, U, Be
4th group: Zn, Mn, Co, Ni
5th group: Ca, Ba, Sr
6th group: Mg, K, Li

Reference books:

Vogel's textbook of semimicro qualitative analysis, 5th Edition by G. Svehla.

Practical-2

ORGANIC CHEMISTRY PRACTICALS - I

Preparation, recrystallization, and determination of melting point & yield of the following compounds:

- | | | |
|-----------------------------------|-----------------------------|--------------------------------|
| (i) Aspirin, | (ii) Nerolin, | (iii) Chalcone, |
| (iv) <i>p</i> -Nitro acetanilide, | (v) 2,4,6- Tribromoaniline, | (vi) <i>m</i> -Dinitrobenzene, |
| (vii) Phthalimide, | (viii) Diels-Alder adduct. | |

Books Suggested

1. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4th & 6th Ed. (Pearson Education Asia).
2. Vogel's Text Book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, 5 Ed. (Longman Scientific & Technical)



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Practical-3

PHYSICAL CHEMISTRY PRACTICALS -I

1. Determination of critical solution temperature of phenol-water system.
2. Effect of added electrolyte on the CST of phenol-water system.
3. Conductometric titration of Strong acid versus Strong base
4. Dissociation constant of weak acid (CH_3COOH) by conductometric method.
5. Conductometric titration of Weak acid vs Strong base.
6. Determination of cell constant
7. Adsorption of acetic acid on animal charcoal or silica gel.
8. Acid-catalyzed hydrolysis of methyl acetate
9. Determination of partial molar volume of solute – H_2O system by apparent molar volume method.



ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
SECOND SEMESTER- SYLLABUS
(With Effective from 2019-20 admitted batch)

Paper- I: GENERAL CHEMISTRY-II

UNIT-1

Basic Quantum Chemistry-III- Hydrogen atom- solution of $R(r)$, $\Phi(\phi)$ and $\Theta(\theta)$ equations. Probability density in orbitals- shapes of orbitals- Perturbation theory- Time independent perturbation theory(only first order perturbation is to be dealt with)- application to ground state energy of Helium atom- Variation principle- applications- calculation of zero-point energy of harmonic oscillator- many electron atom- Hartee-Fock self-consistent field method(qualitative treatment only)

UNIT-II

Molecular symmetry and Group Theory in chemistry: Basic concepts of symmetry and Group theory-Symmetry elements, symmetry operations and point groups- Schoenflies symbols- Classification of molecules into point groups- Axioms of Group theory- Group multiplication tables for C_{2v} and C_{3v} point groups- Similarity transformations- and classes- Representations- reducible and irreducible representations, Mullikan symbols, Orthogonality theorem and its implications, Character table and its anatomy.

UNIT-III

Treatment of analytical data: Accuracy and precision- Classification of errors- Determinate and Indeterminate errors- Minimization of errors- Absolute and Relative errors, propagation of errors-Distribution of Indeterminate errors- Gaussian distribution- Measures of central tendency-Measures of precision- Standard deviation- Standard error of mean- student's t-test- Confidence interval of mean- Testing for significance- Comparison of two means- F-test- Criteria of rejection of an observation- Significant figures and computation rules.

UNIT- IV

Introduction to computer programming- FORTRAN 77: Basic structures and functioning of computer with P.C. as an illustrative example- Main memory- Secondary storage memory- input/output devices- computer languages- operating systems- principles of algorithms-and flow charts-constants and variables- Arithmetic expressions- Arithmetic statements- Replacement statement- IF statement- logical IF and BLOCK IF statements- GOTO statements-subscripted variable and DIMENSION statement. DO statement- Rules for DO statement- Functions and subroutines- Development of FORTRAN statements for simple formulae in chemistry such as Vander Waals equation- pH of a solution- First order rate equation- Cell constant-Electrode potential.

Flowcharts and computer programs for

- Program for the calculation of Cell Constant, Specific Conductance and Equivalence.
- Rate Constant of First order reaction or Beer's law by linear least square method.
- Hydrogen ion concentration of a strong acid solution/Quadratic equation.
- Solution for Vander Waals equation or Hydrogen ion concentration of a monoprotic weak acid
- Standard deviation and Variance of univariant data

References/ Text books:

- Introductory Quantum chemistry: by A.K. Chandra
- Group theory for Chemistry: by A.K. Bhattacharya, 3. Chemical Applications of Group Theory by FA Cotton, 3rd Edition, Wiley Interscience Newyork
- Introductory Group theory for chemists : by George Davidson
- Vogel's text book of quantitative analysis: by Vogel
- Fundamentals of Analytical chemistry: by Skog and West
- Principles of computer programming(FORTRAN 77 IBM PC): by V.Rajaraman
- Basics of computers for chemists: by P.C. Jurs



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Paper- II: INORGANIC CHEMISTRY-II

UNIT-I

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

$\text{Re}_2\text{Cl}_8^{2-}$, $\text{Mo}_2\text{Cl}_8^{4-}$, $\text{Re}_2(\text{RCOO})_4\text{X}_2$, $\text{Mo}_2(\text{RCOO})_4(\text{H}_2\text{O})_2$, $\text{Cr}_2(\text{RCOO})_4(\text{H}_2\text{O})_2$, $\text{Cu}_2(\text{RCOO})_4(\text{H}_2\text{O})_2$, $\text{Cr}_2\text{Cl}_9^{3-}$, $\text{Mo}_2\text{Cl}_9^{3-}$, $\text{W}_2\text{Cl}_9^{3-}$, Re_3Cl_9 , $\text{Re}_3\text{Cl}_{12}^{3-}$, $\text{Mo}_6\text{Cl}_8^{4+}$, $\text{Nb}_6\text{X}_{12}^{2+}$ and $\text{Ta}_6\text{X}_{12}^{2+}$.

Polyatomic clusters – Zintl ions, Chevrel phases.

UNIT-II

Organometallic compounds - 16 and 18 electron rules. Isoelectronic relationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen and nitric oxide complexes. Isolobal relationship – H, Cl, CH_3 , $\text{Mn}(\text{CO})_5$; S, CH_2 , $\text{Fe}(\text{CO})_4$; P, CH, $\text{Co}(\text{CO})_3$. Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene. Catalysis by Organometallic compounds – Homogeneous Catalysis – Alkene hydrogenation – Wilkinson's catalyst, Hydroformylation.

UNIT-III

Metal Ligand equilibria in solution: Stepwise and overall formation constants and their interaction– trends in stepwise constants – factors affecting the stability of metal complexes–Pearson's theory of hard and soft acids and bases (HSAB), chelate effect and its thermodynamic origin, determination of stability constants of complexes–spectrophotometric method and pH–metric method. Reactivity of metal complexes–inert and labile complexes. Explanation of lability on the basis of VBT & CFT.

Bio-Inorganic Chemistry: Metalloporphyrins with special reference to Haemoglobin & Myoglobin. Biological role of alkali and alkaline earth metal ions with special reference to Ca^{2+} . Biological and abiological Nitrogen Fixation.

UNIT- IV

Inorganic Reaction Mechanisms: Substitution reactions of metal complexes – D, Id, Ia and A mechanisms – Ligand replacement reactions of octahedral complexes – Acid hydrolysis – factors affecting acid hydrolysis – Anation and Base hydrolysis of Cobalt(III) complexes. Ligand displacement reactions of square planar complexes of platinum (II). Factors affecting square planar substitution – trans effect (theories).

Electron transfer reactions of complexes – concept of complementary and non-complementary reactions with examples. Inner and outer sphere mechanisms.

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and R.G. Wilkinson, IV Edition, John, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III edition, Harper International Edition, 1983.
3. Organometallic Chemistry-A unified approach by A. Singh and R.C. Mehrotra, Wiley Eastern Ltd.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)
5. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd..
6. Mechanisms of Inorganic reactions in solution by D.Benson, McGraw Hill, London, 1968.
7. Inorganic chemistry by K.F. Purcell and J.C.Kotz, W.B. Saunders company, New York, 1977.
8. Elements of Bioinorganic Chemistry by G.N. Mukherjee and Arabinda Das, U.N. Dhur & sons Pvt. Ltd, Calcutta.



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Paper-III: ORGANIC CHEMISTRY-II

UNIT-I

Reaction Mechanism

15Hrs

(A) *Aliphatic Nucleophilic Substitution and Nucleophilic Aromatic substitution*: Stereochemistry of S_N^2 and S_N1 mechanisms, Neighboring Group Participation (Anchimeric assistance), NGP by O, S, N: Aromatic Nucleophilic substitution: S_N2 (Ar) (Addition – Elimination), S_N1 (Ar) and benzyne mechanisms (Elimination - Addition); evidence for the structure of benzyne. Von Richter Sommelet-Hauser rearrangements.

(B) *Elimination Reactions*: Type of elimination reactions, mechanisms, Stereochemistry and Orientation, Hofmann and Saytzeff rules, Syn elimination versus anti-elimination, competition between elimination and substitution, dehydration, dehydrogenation, dehalogenation, decarboxylative eliminations and pyrolytic eliminations

UNIT-II

Addition Reactions

15 Hrs

(A) *Addition to Carbon – Carbon Multiple Bonds*: Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region and chemo selectivity, orientation and reactivity, Hydrogenation of double and triple bonds, hydrogenation of aromatic rings, Hydroboration.

(B) *Addition to Carbon-Hetero Multiple Bonds*: Steric course of addition reactions to C=O and C=N, Aldol, Cannizzaro, Perkin, Knoevenagel, Claisen- Schmidt, Claisen, Dieckman, Benzoin and Stobbe condensations, Reformatsky reaction, Tollen's reaction, Prins reaction: Wittig, Grignard, Mannich, and Michael reaction.

UNIT-III

Molecular Rearrangements

15 Hrs

Types of molecular rearrangements, migratory aptitude; Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein, Tiffeneau – Demjanov, Dienone – Phenol, Arndt-Eistert synthesis;

Rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements;

Rearrangements to electron deficient oxygen: Baeyer-villiger, Hydro peroxide rearrangement and Dakin rearrangements; Neber rearrangement, Benzil-Benzilic acid and Favorskii rearrangements

UNIT-IV

Spectroscopy and Protecting Groups

15 Hrs

- A. i) U.V. Visible absorption laws, Electronic excitations and absorption shifts
ii) I.R. : Fundamental modes of vibrations in IR Spectroscopy, Finger Print Region and its importance.
iii) NMR: Chemical shift and its importance, Coupling constant and its importance, Factors affecting chemical shift and coupling constant, Deuterium-deuterium exchange and Deuterium Labeling.
iv) Mass: Some useful terms used in Mass spectrometry: Molecular ion, Fragmentation, Cleavage, Rearrangement, Loss of small molecules, Isotope Abundance, Metastable ions, Even-electron rule, Nitrogen rule, McLafferty Rearrangement.
- B. Protection of carbonyl, Hydroxyl, carboxylic and Amine groups

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons).
2. Modern Organic Reactions, H. O. House (Benjamin)
3. Structure and Mechanism in Organic Chemistry C. K. Ingold (Cornell University Press).



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4. Organic Chemistry, Paula Yurkanis Bruice, 4th Ed. (Printice Hall)
5. Organic chemistry-Clayden J. (Oxford)
6. Organic Chemsitry, Wade, L.G. Jr. 5th Ed. (Pearson)
7. Organic Chemistry, Salmons, P.W. & Others, 8th Ed. (John Wiley & Sons)
8. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
9. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row,
10. (Publishers, Inc.).
11. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman).
12. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International).
13. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley). 13. Stereochemistry to Organic Compounds, Nasipuri, 2nd Ed. (New Age International).
14. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International). Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)
15. Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990.
16. Organic Spectroscopy- Second Edition, W.Kemp, ELBS Macmillan, 1987.
17. Applications of absorpition spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
18. Spectrometric identification of Organic Compounds-Fourth Edition, R.M. Silverstein: G.C.Vassiellr and T.C. Merill, Johne Willey, Singapore, 1981.
19. Introduction to spectroscopy-D.L.Pavia, G.M.Lampman, G.S.Kriz, 3rdEd (Harcourt college publishers).



ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
SECOND SEMESTER- SYLLABUS
(With Effective from 2019-20 admitted batch)

Paper – IV: PHYSICAL CHEMISTRY-II

UNIT-I:

Physical methods of molecular structural elucidation: NMR: Principle and theory, Nature of spinning particle and its interaction with magnetic field. Chemical shift and its origin. Spin-Spin interaction, Application of NMR to structural elucidation- Structure of ethanol, dimethylformamide, styrene and acetophenone.

Electron Spin Resonance: Principle and experimental technique- g -factor, line shapes and line widths- hyperfine interactions- applications of ESR studies.

UNIT -II:

Thermodynamics-II- Brief review on entropy; entropy changes accompanying specific process – expansion, phase transition, heating, measurement of entropy. Nernst heat theorem; Third law of thermodynamics- Determination of the absolute entropy- Apparent exceptions to Third law of thermodynamics.

Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law – Partition Function, (Definition and significance): Molar and molecular partitions-translational, rotational, vibrational and electronic partition functions- Relation between thermodynamic functions (E , H , S , G and C_v) and the partition functions

UNIT-III:

Electrochemistry I: Electrochemical cell- Galvanic and electrolytic cell. Concentration cell with and without transference, Effect of complexation on redox potential- ferricyanide/ ferrocyanide couple, Iron (III) phenanthroline / Iron (II) phenanthroline couple. Determination of standard potential, solubility product equilibrium constant and activity coefficients from EMF data.

Bjerrum theory of ion association (elementary treatment) Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required), Calculation of mean ionic activity coefficient; Limitations of Debye-Huckel theory. Effect of dilution on equivalent conductance of electrolytes - Anomalous behavior of strong electrolytes. Debye Huckel-Onsagar equation – verification and limitations, Fuel Cells.

UNIT-IV:

Electrochemistry II: The electrode-electrolyte interface. The electric double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and over-potential. Derivation of Butler-Volmer equation. High field approximation, Tafel equation, Low field equilibrium, Nernst equation. Voltametry-Concentration polarization, experimental techniques

Books:

1. Text book of Physical Chemistry by Samuel Glasstone, McMillan Pub.
2. Physical Chemistry by W.J.Moore, Prentice Hall
3. Physical Chemistry by G.W. Castellon, Narosha Publishing House
4. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
5. Modern Electrochemistry, 2A & 2B, JOM Bockris & A.K.N.Reddy, Plenum publishers
6. Introduction to Electrochemistry, S.Glasstone.
7. Fundamentals of Molecular Spectroscopy, Banwell
8. Spectroscopy by Straw & Walker.



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9. Statistical thermodynamics , M.C.Gupta
10. Statistical Thermodynamics, M.Dole



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LABORATORY WORK (6 hrs/ week)

Practical-1

INORGANIC CHEMISTRY PRACTICALS –II

Quantitative analysis:

Volumetric:

1. Determination of Ferric iron by photochemical reduction
2. Determination of Nickel by EDTA
3. Determination of Calcium and Magnesium in a mixture by EDTA
4. Determination of Ferrocyanide by Ceric sulphate
5. Determination of Copper(II) in presence of iron(III)

Gravimetric:

6. Determination of Zinc as Zinc pyrophosphate
7. Determination of Nickel from a mixture of Copper and Nickel.

Reference books:

Vogel's textbook of quantitative chemical analysis, 5th edition by G.H. Jeffery et al.

Practical-2

ORGANIC CHEMISTRY PRACTICALS –II

Systematic qualitative analysis of an organic mixture containing two compounds

Identification of method of separation and the functional group(s) present in each of them and preparation of one solid derivative for the confirmation of each of the functional group(s).

Practical-3

PHYSICAL CHEMISTRY PRACTICALS –II

1. Distribution of iodine between CHCl_3 and water
2. Distribution of I_2 between CHCl_3 and aq. KI solution- calculation of equilibrium constant.
3. Determination of Coordination number of cuprammonium cation.
4. Titration of mixture Strong acid and weak acid versus Strong base by conductometry.
5. Titration of Strong acid Vs Strong Base – pH – metry.
6. Titration of mixture of ($\text{NaHCO}_3 + \text{Na}_2\text{CO}_3$) Vs HCl – pH- metry.
7. Titration of Strong acid Vs Strong Base using Quinhydrone electrode.
8. Titration of Fe^{+2} Vs $\text{K}_2\text{Cr}_2\text{O}_7$ – potentiometry
9. Verification of Beer-Lambert's law by Iron-thiocyanate system –colorimetry.
10. Determination of single electrode potential of Cu^{2+}/Cu and estimate the given unknown concentration.