



M.Sc. CHEMISTRY CBCS PATTERN IN SEMESTER SYSTEM

DEPARTMENT OF CHEMISTRY

KAKATIYA UNIVERSITY WARANGAL – 506 009

Department of Chemistry, Kakatiya University introduces Choice Based Credit System (CBCS) for M.Sc. (2 Year course) chemistry for the students admitted in M.Sc. Chemistry course from 2016-17 academic year onwards.

Scheme for CBCS, the workload for each paper, distribution of marks, the number of credits and scheme of examination are attached herewith.

Internal Assessment examination will be conducted twice in every Semester. The main examination (theory and practical) will be conducted at the end of each semester.

One open elective in III semester and one is in IV semester are offered by Department of Chemistry for all the PG-students.

Students joined in M.Sc. Chemistry should choose one open elective offered by Department of chemistry or any other Department of Kakatiya University.

The syllabi of theory and practical papers of I, II III, and IV semesters are enclosed. The syllabi of open elective offered in IV semester will be kept available for the next academic year.

- Prof. Gade Dayakar

Chairperson

Board of Studies in Chemistry

II SEMESTER
PAPER-I: INORGANIC CHEMISTRY (2CHT5)
(Marks-100, Total hrs: 60)

Unit I Electronic-spectra of metal complexes:

Free-ion terms and energy levels - Electron configuration, Microstates and Terms. Calculation of microstates for **p** and **d** configurations, Russel-Saunders (L-S) coupling. Derivation of terms for **p²** and **d²** configurations, Ground state term symbols for **d** configurations, Hole formalism, Hund's rules to determine ordering of energy levels, Effect of weak fields on free ion terms, Selection rules governing electron transitions and breakdown of selection rules, Orgel diagrams for **d¹** to **d⁹** systems, Electronic spectra of $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$, $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$, $[\text{V}(\text{H}_2\text{O})_6]^{3+}$, $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$, $[\text{CoF}_6]^{3-}$, $[\text{CoCl}_4]^{2-}$ and $[\text{NiCl}_4]^{2-}$ complexes, Charge transfer Spectra, Calculation of ligand field parameters - Racah parameter (**B**), Crystal field splitting (**10DQ**) and Nephelauxetic ratio (**b**).

Unit II Organometallic Compounds:

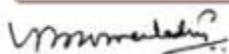
Classification and nomenclature of organometallic compounds, Principles of synthesis of organometallic compounds. Synthesis, structure and properties of organometallic compounds of **Al** and **Sn**. 18-electron rule and stability of organotransition metal compounds. Synthesis, structure and bonding of olefin, allyl and cyclopentadienyl organometallic compounds of **Fe**, **Pd** and **Pt**. Applications of organometallic compounds of **B** and **Si** in organic synthesis. Organometallic compounds in homogeneous catalysis – Hydrogenation, Hydroformylation and Isomerization processes.

Unit III Bioinorganic Chemistry:

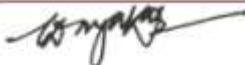
Metal ions in biological systems - Brief survey of metal ions in biological systems, Basic principles underlying biological selection of elements, Physiological effects of metal ion concentration.

Oxygen transport and storage - Haemoglobin and Myoglobin, Geometric, electronic and magnetic aspects of dioxygen binding, oxygen adsorption isotherms and cooperativity, Physiological significance of hemoglobin, Role of globin chain in haemoglobin.

Metals/ Metal compounds in medicine - Introduction, Metal deficiency and disease, Iron deficiency, Zinc deficiency, and Copper deficiency; Metals used for diagnosis and radiodiagnosis; Lithium, Gold and Platinum compounds used in therapy.



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Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,

Unit IV Ligational aspects of diatomic molecules:

Metal Carbonyls: Classification of metal carbonyls, General methods of preparing metal carbonyls, Ligational properties of Carbon monoxide (CO), Donor and acceptor molecular orbitals of CO, Bonding modes of CO, Evidence for multiple bonding, Eighteen electron rule, Electron counting methods i) Neutral atom method and ii) Oxidation state method, Structural and bonding aspects of $\text{Ni}(\text{CO})_4$, $\text{Mn}_2(\text{CO})_{10}$ and $\text{Fe}_2(\text{CO})_9$.

Metal carbonyl clusters- Factors favouring metal-metal bond, Classification of metal carbonyl clusters, Structures of $\text{Fe}_2(\text{CO})_9$, $\text{Co}_2(\text{CO})_8$, $\text{Fe}_3(\text{CO})_{12}$, $\text{Ru}_3(\text{CO})_{12}$, $\text{Co}_4(\text{CO})_{12}$, and $\text{Rh}_6(\text{CO})_{16}$.

Metal nitrosyls: General methods of preparing metal nitrosyls, Donor and acceptor molecular orbitals of nitric oxide (NO), Bonding modes of NO, structural and bonding aspects of $[\text{IrCl}(\text{PPh}_3)_2(\text{CO})(\text{NO})]^+$ and $[\text{RuCl}(\text{PPh}_3)_2(\text{NO})_2]^+$.

Metal dinitrogen complexes - Dinitrogen molecule (N_2) as a ligand, Molecular orbitals of N_2 , Bonding modes - Terminal and Bridging, Structures of Ru (II) and Os (II) dinitrogen complexes.

Recommended books:

1. Inorganic chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed., Harper Collins College Publishers.
2. Introduction to ligand fields, B. N. Figgis, Wiley.
3. Concise Inorganic Chemistry, J. D. Lee, Blackwell Science.
4. Organometallic Chemistry, R. C. Mehrotra and A. Singh, New age international.
5. Metalorganic Chemistry, A. J. Pearson, Wiley.
6. Bioinorganic Chemistry, L. Bertini, H.B. Gray, S. J. Lippard and S. J. Valentine, Viva Low-Priced Student edition.
7. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg.
8. Bioinorganic Chemistry, K. Hussain Reddy, New Age international Publishers.
9. Structure and bonding Vol. 55 H. J. Clark.
10. Modern inorganic Chemistry, W. L. Jolly, McGraw-Hill.
11. Concise coordination Chemistry, R. Gopalan and V. Ramalingam, Vikas Publishing Home Pvt. Ltd.

Paper – V INORGANIC CHEMISTRY PRACTICALS (2CHP4)**I. Estimations:**

1. Glucose by using Fehling's solution
2. Vitamin – C
3. Calcium in Milk
4. Iodine value of Oil
5. Chlorine in Bleaching Powder

II. Analysis of Binary Mixtures:

1. Determination of Cu^{2+} and Ni^{2+}
2. Determination of Fe^{3+} and Al^{3+}
3. Determination of Cu^{2+} and Zn^{2+}
4. Determination of Ca^{2+} and Mg^{2+}
5. Determination of Ferrocyanide & Ferricyanide

Scheme of valuation

Marks: 75

Time: 4Hrs

Standardization Estimation	–	24
of sample Viva, Record	–	36
and samples	–	15

Recommended Books:

1. A Text Book of quantitative inorganic analysis (3rd and 6th editions)

II SEMESTER
PAPER-II: ORGANIC CHEMISTRY (2CHT6)
(Marks-100, Total hrs: 60)

Unit I Named reactions in organic synthesis:

Beckmann rearrangement, Mannich reaction, Michael addition, Dienone-Phenol rearrangement, Robison annulation, Favorski reaction, Baylis-Hillman reaction, Shapiro reaction, Ugi reaction, Grubbs reaction, Heck reaction, Suzuki coupling, Stille coupling, Sonogashira coupling, and Buchwald reaction.

Unit II Stereochemistry II:

Conformational analyses of Cycloalkanes: Conformations of small and medium sized rings and conformations of mono and disubstituted cyclohexanes. Factors governing the reactivity of equatorial and axial substituents attached to the cyclohexane ring – Relative stability and reactivity of conformational diastereomers –Stereochemistry of bicyclic systems involving five and six numbered rings. Conformations of cyclohexanone - Stereochemistry of addition to the carbonyl group in rigid cyclohexanone system.

Use of physical methods (dipole moment, IR and NMR) in determining the preferred conformers of simple organic molecules such as 1,2-dihalo ethanes, halohydrins and vicinal diols.

ORD studies: Optical rotation and optical rotatory dispersion, axial haloketone rule, octant rule, applications of ORD studies in the determination of configuration and conformation of organic molecules.

Unit III Protection of functional groups and Nucleic acids:

Protection of functional groups: Principles of (1) protection of alcohols – Ether formation: methyl, benzyl, allyl, methoxy ethoxy methyl (MEM), THP, silyl, and TBDMS ethers; Ester formation– methyl, benzoyl, tosyl, and p-nitro benzoyl ester (2) protection of diols – acetal, ketal and carbamate formation (3) protection of carboxylic acids – Ester formation: methyl, benzyl, t-butyl, p-nitrobenzyl, p-bromophenacyl, and silyl esters (4) protection of amines – Amide and Carbamate formation with formyl, acetylation, benzoyl, benzyloxy carbonyl (CBZ), *tert*-butyloxycarbonyl (BOC), *tert*-butyl azido formyl, phthaloyl, di-*tert*-butyl pyrocarbonyl, Fluorenylmethyloxycarbonyl (Fmoc), and triphenyl methyl groups (5) protection of carbonyl groups – acetal, ketal, 1,3-dioxolane, 1,3-dioxane, 1,3-dithiolane, 1,3-oxathiolane and 1,3-dithiane formation.

Nucleic acids: Isolation, structure, and properties of RNA & DNA – synthesis of nucleosides, nucleotides, and synthesis of polynucleotides. Biosynthesis of RNA and DNA.

Unit IV Nonbenzenoid aromatic compounds:

Concept of aromaticity, Robinson's sextet theory, Huckel's rule, basis for the Huckel's rule, limitations of the Huckel's rule- Alternant and Non-alternant hydrocarbons Craig's rule – Various Nonbenzenoid aromatic molecules – Synthesis and properties of aromatic 3,4,5,6,7,8-membered rings, metallocenes, annulenes, heteroannulenes, azulenes, fullerenes(C_{60}), Sydnones – Antiaromatic compounds,

Recommended Books:

1. Reaction mechanisms – Jerry March
2. Organic Chemistry – Volume-I & II – I.L. Finar
3. Carbohydrate chemistry – Davidson
4. Textbook of organic chemistry – Morrison and Boyd
5. Organic reagents – Fieser and Fieser
6. Modern textbook of organic chemistry – Furguson

Paper - VI ORGANIC CHEMISTRY PRACTICALS (2CHP5)

Identification of Organic compounds – Systematic qualitative analysis:

Physical data – Boiling points/ Melting points; Ignition test, Solubility classification, Detection of extra elements N,S and Halogens (Lassaigne sodium fusion test, Beilstein test). Functional group tests and preparation of two rational derivatives - determine the melting points of solid derivatives and reference to literature to identify the compounds. A minimum of eight following compounds to be studied as unknown covering at least one from each of the solubility classes.

List of suggested compounds:

Glucose, Fructose, Benzaldehyde, p-Anisaldehyde, p-Chlorobenzaldehyde, Acetophenone, p-Nitroacetophenone, Benzophenone, Benzoic acid, p-Nitrobenzoic acid, p-Chlorobenzoic acid, Anisic acid, Phenol, p-Cresol, b-Naphthol, p-Chlorophenol, Aniline, p-Toluidine, p-Anisidine, o-Chloroaniline, m-Chloroaniline p-Chloroaniline, Diphenylamine, N-methyl aniline N,N-dimethyl aniline, Benzamide, Ethyl benzoate, methyl benzoate, Nitrobenzene, Chlorobenzene, Bromobenzene, Naphthalene and Anthracene, Biphenylanthracene.

Scheme of valuation

Marks: 75

Time: 4Hrs

Determination of M.P/ B.P, Extra element test, Solubility test	– 18
Functional group test	– 24
Preparation of derivatives	- 18
Viva, Record and samples	– 15

Recommended books:

1. Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2. Practical Organic Chemistry - Frederick George Mann and Bernard Charles Saunders

II SEMESTER

PAPER-III: PHYSICAL CHEMISTRY (2CHT7)

(Marks-100, Total hrs: 60)

Unit I Thermodynamics – II:

Statistical Thermodynamics: Thermodynamic probability of distinguishable and indistinguishable particles-most probable distribution–entropy and probability (Boltzmann–Planck equation), Maxwell–Boltzmann distribution law–partition function and types. Translational, rotational, vibrational and electronic functions–Relation between thermodynamic functions (E, H, S and G) and partition functions-factorization into translational, rotational, vibrational and electronic contributions of monoatomic and diatomic molecules. Sackur-tetrode equation of entropy. Equilibrium constant.

Quantum Statistics: Basic concepts of quantum statistics–Bose–Einstein and Fermi-Dirac statistics–comparison with Maxwell–Boltzmann statistics.

Unit II Solid State:

Bonding in metals: Valence bond theory of metallic bond, Free electron Theory-Molecular orbital approach to the Band theory of solids–classification of solids–Insulators, conductors, and semiconductors–types of semiconductors, temperature effect on conductivity, photoconductivity and photovoltaic effect–p and n junctions.

Defects in crystals: Point defects, colour centers, line defects and plane defects.

Superconductivity: Superconductivity and types of superconductors – Theories of superconductivity – BCS theory – Applications of superconductors. High temperature superconductors - Structure of defect perovskites. High superconductivity in cuprates.

Specific heats of solids: Dulong and Petit's law, Einstein theory and Debye theory of specific heats. **Solid state reactions:** Classification and theory of solid state reactions D-Wagner's theory - examples.

Unit III Chemical Kinetics - II:

Effect of substituent on the rate of reaction – Hammett's and Taft's equations– use of ρ and r constants and extended Hammett equation. Yukawa–Tsuno equation–Nonlinear Hammett's Plots–Isokinetic temperature and its determination.

Acid-base catalysis: Homogeneous acid–base catalysis–mechanism of acid-base catalysis-protolytic and prototropic mechanism.

Enzyme catalysis: Specific action and classification of enzymes–Kinetics and mechanism of single substrate reaction–Michaelis–Menten Kinetics. Production detection and estimation of free radicals.

Chain reactions: General Characteristics–Kinetics of Chain reactions–Mechanisms of thermal reaction of hydrogen with chlorine and bromine and their rate expressions–thermal decomposition of N_2O_5 and C_2H_6 -general kinetic schemes-Inhibition of chain reactions by NO.

Unit IV Quantum Chemistry - II:

Rigid rotator: Application of Schrodinger equation to rigid rotator– derivation of energy expression and wave function of a rigid rotator–solution of (j) and (q) parts of wave functions–total wave function of rigid rotator.

Hydrogen atom: Separation of (r), (j) and (q) equations–Solution of radial equation– Total wave function for hydrogen atom–radial and angular plots–probability functions and radial probability density plots for 1s and 2s orbitals.

Approximation methods: Variation method–principle and its application to hydrogen atom–perturbation method–First order correction terms of energy and wave function– application to particle in a one-dimensional box under an electric field.

Bonding in molecules: Born-oppenheimer approximation - construction of molecular orbitals by LCAO. MO theory of H_2^+ ion. Energy and wave function expressions (no derivation). Basic postulates of Huckel's p electron theory and its applications to ethylene system.

Recommended books:

1. Physical Chemistry by Donal D; Mcquarrie & John D Simon.
2. Atomic Structure and the Chemical Bond including Molecular Spectroscopy –Manas Chanda (4th edn)
3. Physical Chemistry - Peter Atkins and de Pulpa Oxford University Press.
4. Principles of Physical Chemistry - Samuel H. Maron and Carl F. Prutton.
5. Advanced Physical Chemistry -Gurdeep Raj Goel Publishers House, Meerut.
6. Quantum Chemistry - R.K.Prasad
7. Thermodynamics - Samuel Glasstone
8. Chemical Kinetics by K.J. Laidler
9. Chemical Kinetic Methods–Principles of Relaxation techniques & Applications - C. Kalidas.
10. Principles of Chemistry by Paul Ander Anthony J. Sonnessa.
11. Solid State Chemistry -D.K. Chakravarty
12. Solid state chemistry and Applications - A.R. West, Plenum Press.
13. Solid State physics - S.O. Pillai, New Age Publishers.

Paper – VII PHYSICAL CHEMISTRY - PRACTICALS (2CHP6)

1. Potentiometry:

a. Acid –base titrations:

- (i) Strong acid with strong base.
- (ii) Weak acid with strong base and determination of P^{ka} of weak acid.
- (iii) Mixture of acids with strong base.

b. Redox titrations:

- (i) Ferrous ion with $KMnO_4$ or $K_2Cr_2O_7$
- (ii) Ferrous ion with Ce^{+4}

c. Precipitation titrations:

- (i) KCl or KI with $AgNO_3$
- (ii) Mixture of ($KCl + KI$) with $AgNO_3$

2. Colorimetry:

Verification of Lambert-Beer's law and determination of molar extinction coefficient of $KMnO_4$, $CuSO_4$, $K_2Cr_2O_7$, $Cu(NH_4)_6SO_4$

- 3. Verification of Freundlich adsorption isotherm-Acetic acid-activated charcoal system
- 4. Distribution of Iodine between CCl_4 and aqueous KI . (determination of unknown concentration of KI)
- 5. Determination of partial molar volume of methanol in aqueous methanol.

Scheme of valuation

Marks: 75

Time: 4Hrs

Experiments (2)	-	30+30 –	60
Viva, Record and samples		–	15

Recommended Books:

- 1. Practical Physical Chemistry -A. Findlay, Longman-London.
- 2. Practical Physical Chemistry -B. Vishwanathan and P.S. Raghavan,
- 3. Practical Physical Chemistry - B.D.Khosla and V.C. Garg. R.Chand & Co. Delhi.
- 4. Systematic Experimental Physical Chemistry by S.W. Raj Bhoj and Dr. T.K. Chondhekar, Anjali Publications, Aurangabad.

II SEMESTER

Paper-IV: Spectroscopy (2CHT8)

(Marks-100, Total hrs 60)

Unit I Symmetry & Group Theory:

Introduction- concepts of symmetry in molecules, symmetry elements, symmetry operations, mathematic rules of a group – abelian and non-abelian groups. Point groups- classifications of point groups- Exercises on molecular point groups -H₂O, o-C₆H₄X₂, C₅H₅N, CH₃Cl, H₂O₂, CH₄, B(OH)₃, C₂H₂Cl₂, [PtCl₄]²⁻, C₃H₄(Allene), [FeCl₆]³⁻, Metallocenes (Eclipsed and Staggered). Descent in symmetry of molecules with substitution (H₂O, HOD, CH₄, CH₃X). Symmetry criteria of optical activity, Symmetry restrictions of dipole moment, group multiplication table – subgroups.

Unit II Microwave & Electronic Spectroscopy:

Microwave spectroscopy: Types of molecular energies and molecular spectroscopy. Classification of molecules based on moment of inertia. Rigid rotator model, energy levels and selection rules of rotational spectra - Calculation of bond lengths of heteronuclear diatomic molecules, Intensity of spectral lines - Boltzmann distribution law-degeneracy of energy states, Effect of isotopic substitution-abundance of isotopes. Nonrigid-rotator, energy levels and its spectrum, Stark effect, Centrifugal distortion constant, Rotational spectra of linear triatomic (like OCS and HCN) molecules.

UV & Visible (Electronic) Spectroscopy: Origin of electronic spectra, Lambert-Beer's absorption law, Types of electronic transitions. Effect of solvent, substituent, conjugation on electronic transitions. Benzene and its substituted derivatives. Applications of UV-visible spectroscopy in analysis (qualitative/quantitative) of polyenes/aromatic (hetero & homo) systems, geometrical isomers, keto-enol tautomers, components of a mixture, ionization constants of acids and bases. Woodward-Fieser rules for calculating absorption maximum in dienes, trienes and a,b-unsaturated carbonyl compounds. Charge transfer spectra of complexes. Photometric titrations. Determination of composition of complexes by Job's slope ratio method. UV spectra of Mesityl Oxide, Phenol and Benzoic acid.

Unit III Infrared and Raman Spectroscopy:

Infrared spectroscopy: Vibrational energy of a diatomic molecule-an harmonic oscillator –Selection rules- Overtones-hot bands. Zero-point energy-Calculation of force constant of diatomic molecules. Rotational –Vibrational spectra of diatomic molecules- P,Q,R branches. Instrumentation–sources-sampling techniques. Normal modes of

vibrations for linear and non-linear molecules (stretching, bending, scissoring, rocking, twisting, wagging). Functional group frequencies-Factors influencing vibrational frequencies-Coupled vibrations and Fermi resonance-combinational bands. Applications of infrared spectroscopy-structure elucidation of simple organic molecules-benzene and its substituted derivatives-cis-trans isomers and keto-enol tautomers. Hydrogen bonding, isotopic effect - study of metal-ligand bonding in complexes. IR spectra of Ethyl alcohol, Acetophenone, Mesityl oxide, Benzaldehyde, Aniline, and Acetaldehyde. **Raman spectroscopy:** Raman effect-Quantum theory-selection rules-Rotational and Vibrational Raman effect. Instrumentation, Mutual exclusion principle and Raman spectra of Hg_2^{2+} , NO_3^- , ClO_3^- , N_2O , CO_2 and CH_4 .

Unit IV NMR Spectroscopy and ESR Spectroscopy:

Nuclear magnetic resonance spectroscopy (NMR): Theory of NMR-Nuclear energy levels-Instrumentation-Relaxation phenomenon, spin-spin and spin-lattice relaxations. Shielding and deshielding mechanism-chemical shift. Factors affecting the chemical shift. Isotropic and anisotropic effects-alkanes, olefins, acetylenes and aromatic systems. Low and High resolution of NMR spectrum of ethyl alcohol. Spin-spin coupling of strongly and weakly coupled systems-coupling mechanism, types of coupling constants. Factor affecting coupling constants-hybridization-dihedral angle and steric effects. NMR spectra of vinyl chloride, acetophenone, monosubstituted benzenes (benzaldehyde, ethylbenzene, p-chloroaniline and benzoic acid). Applications of NMR spectroscopy-hydrogen bonding, keto-enol tautomers, cis-trans isomers, conformational analysis and deuterium exchange reactions.

Electron spin resonance spectroscopy (ESR): Introduction-Principles involved in ESR spectroscopy. Instrumentation, presentation of ESR spectra, hyperfine coupling constant. ESR spectrum of hydrogen atom. Lande's splitting factor and its significance. ESR spectra of organic radicals like methyl, ethyl, isopropyl, benzene (anion and cation radicals), 1,4-benzosemiquinone and naphthalene anion.

Recommended Books:

1. Chemical Applications of Group Theory - F. A. Cotton.
2. Atomic structure and chemical bonding – Manas Chanda (Tata McGraw Hill).
3. Fundamentals of Molecular spectroscopy-Banwell & McCash (Tata McGraw Hill).
4. Molecular spectroscopy-Patel and Patel (Sardar Patel University Press).
5. Spectroscopy organic compounds-P. S. Kalsi (New Age International).
6. Organic Spectroscopy-Jag Mohan (Narosa)

7. Elementary Organic Spectroscopy-Y.R. Sharma (S.Chand & Company).
8. Organic spectroscopy-W. Kemp (ELBS).
9. Nuclear Magnetic Resonance: Basic Principles - Atta ur Rahman.
10. Introduction to Spectroscopy - Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan.
11. Spectroscopy - Donald L. Pavia, Gary M. Lampman, George S. Kriz.
12. Instrumental methods of chemical analysis-G. R. Chatwal & S. K. Anand (Himalaya).
13. Group Theory and Molecular spectroscopy-K. Veera Reddy.
14. Spectrometric Identification of organic compounds, 6th Ed. Rober M. Silverstein & Francis Webster.
15. Applications of spectroscopy-J. Dyer.

