PROF. S. JYOTHI
Chairperson
Board of Studies in Chemistry

NO: 687
27/10/23

DEPARTMENT OF CHEMISTRY
University College
Kakatiya University
Hanumakonda - 506 009, T.S.

Re-Accredited with "A+" Grade by "NAAC"

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No.104 /Chem/KU/2022 Date: 27-10-2023

To

The Registrar
Kakatiya University
Hanumakonda - 506 009

(Through Proper Channel)

Sub: Submission of Pre-Ph.D. Coursework Syllabi Approval - Regd.

Sir,

I am writing to formally submit the approved Pre-Ph.D. Coursework Syllabi for the academic year 2022-2023. These syllabi were reviewed and approved during the Board of Studies, Chemistry meeting held on 15-09-2023, at 3:30 PM.

Please find the enclosed syllabi documents for your records and further processing.

Thanking you

JSM 27.10.23.

Yours faithfully

(Prof. S. Jyothi)
Chairman, Board of Studies
Dept. of Chemistry
KAKATIYA UNIVERSITY
Warangal-506 009 (T.S.) India

Forwarded to Academic Section
J.M.Reddy
28/10/23
(Dean, Faculty of Sciences)

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DEPARTMENT OF CHEMISTRY: KAKATIYA UNIVERSITY – WARANGAL

Pre-Ph. D. Syllabus (Course Work w. e. f. 2023-2024)

PAPER – I: RESEARCH METHODOLGY

(Common for all Specializations)

SECTION-A

Unit-I: Research Design & Ethics

a) **Objectives and types of research**: Motivation in research. Approaches and significance of research. Research and scientific methods. Selecting the problem. Technique involved in defining a problem (hypothesis). Interpretation and report writing. Significance of report writing. Different steps in writing report. Stages of writing. Designing illustrations, tables, figures, general guidelines for illustrations. Thesis writing, Project proposal writing, project process document preparation, Oral presentation. Citation methods, Scopus Indexing, Impact factor, Immediacy index, H-index.

b) **Research Ethics**: Ethics in research. Misconduct and consequences. Forms and consequences of plagiarism. Intellectual property rights. Copy right regulations and patents. Software tools(Turnitin, Urkund, and Ouriginal)

Unit-II: ICT in Research and Data Analysis

a) **Use of ICT for research purposes** – Internet and web-based resources. Search engines. Advanced search techniques. Use of web as a tool for scientific literature survey.

b) **Data Analysis** – Types of errors. Accuracy and Precision. Least square analysis, average and standard deviations. Correlation and Regression analysis**.** Methods of least squares. Regression versus correlation. Correlation versus determination. Types of correlation and their specific applications.

SECTION-B

Unit-III: Separation Techniques

a) **Chromatography:** General discussion. Principle of analytical separation – plate theory, rate theory. Process Optimization, Retention analysis, Resolution. Principles, processing and applications of Gas chromatography, Liquid chromatography, Ion-exchange chromatography, Size exclusion chromatography and Super critical fluid chromatography.

b) **Solvent Extraction:** Principle, Factors favoring solvent extraction of inorganic species into organic phase. Liquid-liquid extraction, Solid-liquid extraction, super critical fluid extraction and their applications.

Unit-IV: Infrared, Raman and Electronic Spectroscopy

a) **Infrared Spectroscopy:** Vibrational energy of a diatomic molecules. Anharmonic oscillator. Selection rules, Overtones, Hot bands, Zero point energy. Calculation of force constant of diatomic molecules. Rotational—Vibrational spectra, P, Q, R-branches. Instrumentation. Sampling techniques. Functional group frequencies. Factors influencing vibrational frequencies, Coupled vibrations, Fermi resonance, Combination bands. Applications of IR Spectroscopy in structure elucidation of organic molecules; cis-trans isomers, keto-enol tautomers, hydrogen bonding. IR spectra of simple molecules.

b) **Raman Spectroscopy:** Raman effect, Quantum theory, Selection rules, Rotational and Vibrational Raman effect. Instrumentation. Mutual exclusion principle. Raman spectra of Hg^{2+}, NO_3^-, ClO_3^-, N_2O, CO_2 and CH_4.

c) **Electronic Spectroscopy:** Origin of electronic spectra, Lambert-Beer's law—its limitations and applications. Types of electronic transitions. Effect of solvent, substituent and conjugation on electronic transitions. Applications of UV-visible spectroscopy (qualitative and quantitative). Cis-trans isomers, Keto-enol tautomers, ionization constants of acids and bases. Photometric titrations. Determination of composition of complexes by Job's slope ratio method. Charge-transfer spectra of complexes.

Unit-V: NMR, ESR and Mass Spectroscopy

a) **NMR Spectroscopy:** Theory of NMR. Shielding and de-shielding mechanism. Chemical shift. Factors affecting the chemical shift. Isotropic and anisotropic effects – alkanes, olefins, acetylenes and aromatic systems. Types of coupling constants. Factors affecting coupling constants. Applications of NMR

PAPER – II: INORGANIC CHEMISTRY

SECTION-A

Unit – I: Coordination Chemistry – I: Bonding and electronic Spectra of Metal Complexes:

(a) Crystal Field Theory and its Limitations; Molecular Orbital Theory & Ligand Field Theory – Symmetry classification of metal and ligand orbitals in cubic and non-cubic environments; octahedral, square planar and tetrahedral geometries; Concept of ligand group orbitals; Molecular Orbital Energy level Diagrams for O_h, D_{4h} and T_d metal complexes with σ and π bonding contribution.

(b) Electronic Spectra: Ligand field terms, Orgel diagrams for $d^1 – d^9$ configurations; Tanabe & Sugano diagrams for d^2 and d^6 configurations; Jahn-Teller Effect – Crystal Field Spectra of O_h and T_d metal complexes of 3d metals; Calculation of 10Dq values, Racah and Nephelauxetic parameters; Charge Transfer Spectra.

Unit – II: Coordination Chemistry – II: Stabilities of Metal Complexes and Host-Guest Chemistry:

(a) Stabilities of metal complexes in solution; Stepwise and overall stability constants; Determination of stability constants by spectrophotometric and pH-metric methods; Factors affecting the stability of metal complexes (Metal and Ligand factors); chelate effect, macrocyclic effect and cryptate effect.

(b) Host-Guest Chemistry: Ligands for binding cations, anions and neutral molecules; Macrocyclic ligands and Cryptands; Types of interactions in Host-Guest complexes, Importance of supramolecular interactions in biology and chemistry; Molecular self-assembly; Molecular sensors.

SECTION-B

Unit – III: Instrumental Methods of Analysis:

(a) Electrometric Methods: polarography and cyclic voltametry:

(b) Thermal methods of Analysis: Principle and instrumentation techniques of Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC). Interpretation of TG curves; factors affecting TG curves. Complimentary applications of TGA, DTA and DSC.

(c) Atomic Absorption Spectrometry (AAS): Principles of AAS, Instrumentation – Flame and Furnace Atomic Absorption Spectrometers; Sensitivity and detection limits in AAS; Interferences – chemical and spectral. Applications of AAS in qualitative and quantitative analysis.

Unit – IV: Bioinorganic Chemistry:

(a) Metalloenzymes: Zinc enzymes – Structural and mechanistic aspects of Carbonic anhydrase, Carboxy peptidase; Role of Zinc; Iron enzymes – Structural and mechanistic aspects of Cytochrome P_{450}, Cytochrome oxidase and peroxidise; Role of Iron. Metalloporphyrins: Hemoglobin – structure, dioxygen binding and transport; physiology of haemoglobin; Synthetic oxygen carriers,

(b) Metal ions in protein folding: Selection and insertion of metals for protein sites; Metal ion folding and cross linking of biomolecules; Calcium and Zinc binding domains in nucleic acids; Protein binding to metallated DNA.

Unit – V: Organometallic Chemistry:

(a) Organometallic compounds of transition metals: metal carbon bond and hapticity; 18 electron rule – Importance in stabilizing structures and reactivities of organotransition metal complexes; General methods of preparation of organotransition metal complexes. Applications of organotransition metal complexes in organic synthesis.

(b) Organometallic compounds in homogenous catalysis: Catalytic reactions and the valence electron (16 vs 18) rule; Oxidative addition, reductive elimination and α and β elimination reactions; detailed study of – hydrogenation; olefin oxidation (Wacker's process); Oligomerization and Polymerization reactions (Ziegler-Natta Catalysis).

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PAPER – II: ORGANIC CHEMISTRY

SECTION-A

Unit-I: Heterocycles

Synthesis and reactivity of isoxazoles, imidazoles, thiazoles, oxazoles, benzimidazoles, quinolines, acridines, 1,8-Naphthyridines, Coumarins, Quinazolines, Quinoxalines, Cinnolines.

Unit-II: Natural Products

Synthesis and structural elucidation of the following compounds.

a) Alkaloids : Reserpine, Narcotine.
b) Terpenoids : Squalene, Zinzeberine
c) Flavonoids : Quercetin, Cyanidin Chloride.
d) Polypeptide enzymes : Insulin, Oxytocin, Biosynthesis of Amino acids.
e) Nucleic acids : DNA & RNA.

SECTION-B

Unit-III: Modern Synthetic Reagents

Di-imide, Thexylborane, Trimethylsilyl chloride, Merrifield resins/solid phase polypeptide synthesis, Phase transfer catalysts, Crown ethers, Lithium dialkyl cuprates. N-Bromosuccinimide, 1,3-Dithanes, Umpolung effect, examples. Allylic oxidation & hydroxylation with SeO_2, tri-n-butyl tin hydride (TBTH), Woodward-Prevost hydroxylation, Baker's yeast. Mc Murray Reaction.

Unit-IV: Pericyclic Reactions

Orbital representation of molecular orbitals. Understanding of bonding, non-bonding orbitals and anti bonding. Symmetry properties of molecules with 2, 3, 4, 5, 6 & 7 contiguous sp^2 carbon systems with special reference to plane of symmetry and two–fold simple axis of symmetry. Electrocyclic reactons of (4n) and (4n+2) electron systems. OCD method: Cycloadditions, 4n and 4n+2 systems— OCD method. Endo preference to Diels-Alder reaction. (1,3), (1,5), (1,7) Sigmatropic rearrangements, Cope and Claisen rearrangements, Sommlet-Hauser rearrangement. FMO approach for Electrocyclic reactions, Cycloadditions and Sigmatropic rearrangements. Elementary treatment of PMO approach to explain Pericyclic reactions. Exercises based on Pericyclic reactions.

Unit-V: Combined applications of UV, IR, NMR and Mass Spectra

Analytical approach towards the structure elucidation of organic molecules by combined applications of UV, NMR, IR and mass spectra.

References:

1. Heterocyclic Compounds – R. K. Bansal.
2. Heterocyclic Chemistry – Jack & Smith.
3. Organic Synthesis – O. House.
4. Organic Synthesis – Michael Smith.
5. Pericyclic reaction – Mukherjee & Singh.
6. Spectrometric identification of organic compounds – Silverstein, Bassler & Morill.
7. Photochemistry & Pericyclic reactions – Jagadamba Singh & Maya Singh.
8. Organic Spectroscopy – Jag Mohan.
9. Organic Chemistry Vol.II – I. L. Finar.
10. Terpenoids – Mayo.
11. Alkaloids – Benteley.
12. Reagents – Fieser & Fieser.

***Note: Examination Pattern.**
Section-A: Four questions. (Two questions from each unit).
Section-B: Six questions: (Two questions from each unit).
The candidate has to answer any five questions choosing at-least one from each section.

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Spectroscopy, hydrogen bonding, keto-enol tautomers, cis—trans isomers, conformational analysis, deuterium exchange reactions. Spin-spin coupling to structure and stereochemistry of organic molecules. NOE and its applications. Lanthanide shift reagents. Applications of CMR spectra. ^{13}C Chemical shifts and factors affecting the chemical shifts – Applications of CMR spectrosocopy.

b) **ESR Spectroscopy:** Introduction. Principles involved in ESR spectroscopy. Instrumentation. Presentation of ESR spectra. Hyperfine coupling. ESR spectrum of hydrogen atom. Lande's splitting factor and its significance. ESR spectra of radicals like methyl, ethyl, isopropyl, bezene(anion & cation), 1,4-bezosemiquinone and naphthalene anion. Zero field splitting and Kramer' s degeneracy. Applications of ESR spectroscopy.

c) **Mass Spectroscopy:** Ionisation of molecules (electronic and chemical ionization). Instrumentation. General patterns of fragmentation. Applications of mass spectroscopy in the structural determinations. Fragmentation pattern in different functional group systems and individual heterocyclic systems (Furan, Pyrrole, Thiophene and Pyridine).

References:

1. Research Methodology: Methods and techniques - C. R. Kothari, 2nd Edn, (New Age International Publishers).
2. Research methodology and statistical tools – P. Narayana Reddy and G. V. R. K. Acharyulu. Ist Edn, (Excel books, New Delhi, 2008).
3. Statistical Methods – S. P. Gupta. (S. Chand & Sons, New Delhi, 2005).
4. R. Ganeshan. Research Methodolgy for Engineers (MJP Publications, 2011).
5. Principles of Instrumental analysis, 5th edition. Skoog (Hollar and Nieman Harcourt, Asia).
6. Vogel's text book of quantitative chemical analysis 6th Edn. Mendham, Denney, Barnes and Thomas. Low Price edition.
7. Spectroscopy of organic compounds – P. S. Kalsi (New Age International).
8. Organic spectroscopy – Jag Mohan (Narosa Publishers)
9. Elementary Organic Spectroscopy – Y. R. Sharma (S. Chand & Company).
10. Molecular Spectroscopy – William Kemp (ELBS).
11. Applications of Spectroscopy – J. Dyer
12. Fundamentals of Molecular Spectroscopy – Banwell & M C Cash (Tata Mc Graw Hill)

***Note: Examination Pattern.**
Section-A: Four questions. (Two questions from each unit).
Section-B: Six questions: (Two questions from each unit).
The candidate has to answer any five questions choosing at-least one from each section.

13. Hilary et. Glasman Dead, Science Research Writing, Imperial College Press.
14. https://www.wikipedia.org.

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Reference Books:

1. Advanced inorganic chemistry; F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6th edn. (Wiley Interscience, NY 1999).
2. Inorganic Chemistry, J. E. Huhey, K. A. Keiter and R. L. Keiter, 4th edn. (Harper Cottens College Publications, 1993).
3. Inorganic Chemistry; K. F. Purcell and J .C. Kotz, Holt-Saunders. (International Edn, London 1977).
4. Symmetry and spectroscopy of molecules; K. Veera Reddy, 2nd edn. (New Age International Ltd.)
5. Electronic spectroscopy; A. B. P. Lever.
6. Infrared and Raman spectroscopy of inorganic and coordination compounds, K. Nakamoto
7. Structural methods in Inorganic Chemistry; E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS
8. Physical methods in Chemistry; R. S. Drago, (Saunders College Publishing, 1977).
9. Principles of instrumental analysis; Skoog, Holler and Wieman, (Harcount Asia Pvt Ltd.)
10. Instrumental methods of analysis; Willard, Dean and Settle
11. Principles and Practice of Analytical Chemistry; F. W. Fifield & D. Kealy (Backwell Science Ltd.)
12. Principles of Bioinorganic Chemistry; S. J. Leppard and J. M. Berg.
13. Bioinorganic Chemistry; Bertini, Gray, Lippard and Valentine.
14. Inorganic biochemistry; J. A. Cowan, (VCH Publications).
15. Supramolecular Chemistry; J. M. Lehn.
16. Core concepts in Supramolecular Chemistry and Nanochemistry; J. W. Steed, D. R. Turner and K. Wallace, Wiley 2007.
17. Principles and applications of organotransition metal chemistry; Collman.
18. The Organometallic chemistry of transition metals; Crabtree.
19. Metalloorganic chemistry; Pearson.
20. Homogenous catalysis by metal complexes; M. M. Taqui Khan and A. E. Martel, Vol. I & II.
21. Homogenous catalysis; G. W. Parshall, John Wiley & Sons, New York.

***Note: Examination Pattern.**

Section-A: Four questions. (Two questions from each unit)**.**

Section-B: Six questions: (Two questions from each unit)**.**

The candidate has to answer any five questions choosing at-least one from each section.

PAPER-III: PHYSICAL CHEMISTRY
SECTION -A

Unit-I: Quantum chemistry

(a) Exact quantum mechanical results:

Time-independent Schrodinger equation, Postulates of quantum mechanics, Operator concept, quantum mechanical operators in Cartesian and Spherical polar co-ordinate systems, some properties of quantum mechanical operators. Review of particle in a box problem. Harmonic oscillator, rigid rotator. Tunneling effect, Born-Oppenheimer approximation, Solution of the Hydrogen- like atom, radial and angular wave functions.

(b) Angular momentum and electronic structure of atom

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Wave functions of poly-electron atoms, Slater determinant. Atomic term symbols, term separation of pn and dn configurations, spin-orbit coupling, Zeeman splitting.

(c) approximation methods

The Variation theorem, linear variation principle, application to hydrogen atom and helium atom. Perturbation theory -first order(non-degenerate & degenerate). Application of perturbation method to helium atom.

(d) Chemical Bonding

LCAO-MO approximation, H_2^+molecular ion, brief introduction to H_2. Molecular term symbols. Valence bond treatment of H_2, comparison of M O and V B methods in the light of H_2 molecule. Hybridization of orbitals (sp, sp2 & sp3). Huckel's Pi-MO theory of conjugated systems; Application to linear and cyclic

polyenes . Pi-electron charge and bond-order. Alternant hydrocarbons, heteroatomic conjugated systems. Limitations of Huckel theory and improvement.

Unit-II:Thermodynamics of electrolyte solutions

(a) Ion solvent Interactions: Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) treatments of ion-solvent interactions.

Ion-Ion Interactions: Activity and activity co-efficients. Debye-Huckel theory of activity coefficients of electrolyte solutions; derivation of Debye-Huckel limiting law, validity and extension to high concentrations; ion-pair formation-Bjerrum model. Debye- Huckel-Onsager conductance equation and brief idea of its extension.

(b) Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Derivation of Boltzmann distribution law. Bose-Einestein and Fermi-Dirac distribution equations (without derivation) and comparison of the three statistics. Partition function & its significance. Translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions , application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions.

(c) Irreversible Thermodynamics

Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity. Gibb's equation , entropy production, entropy production due to matter flow, heat flow, charge flow & chemical reactions. Concept of forces & fluxes, Onsagers theory of irreversible processes- phenomenological laws, their domain of validity. Chemical reactions near equilibrium. Transformation properties of forces and fluxes. Electrokinetic phenomena.

Unit-III: Electrochemistry

Electrified interface, concept of surface excess. Thermodynamics of electrified interface, lipman equation, electrocpillary curves. Methods for determination of surface excess Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models.Ionic Adsorption at electrodes – isotherms for adsorption (Langmuir, Frumkin and Temkin isotherms) Adsorption of organic molecules – an introduction Electron transfer at electrified interface at and away from equilibrium. Derivation of Butller-Volmer equation, low and high field approximations, Introduction to corrosion mechanism and types of corrosion, corrosion current and corrosion potential. Electrodics of corrosion in absence of oxide layer, monitoring of corrosion, and inhibiting corrosion.

Unit-IV:Chemical kinetics

General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis. Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory Dynamics of unimolecular reactions (Lindman-Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces. Surface Reactions: Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langnuir- Riedel mechanism], classical & statistical treatments. Ionic Reactions: Single & duble sphere models of ionic reactions. Diffusion controlled reactions (partial & full microscopic iffuion control) Chain Reactions: Thermal Hydrogen-Bromine reaction, explosive reactions, oscillatory reactions (BZ reaction)

Unit-V: Surface Chemistry

(a) Crystal defects and solid state reactions

Various classifications of crystal defects. Thermodynamics of Schottky & Frankel defects.Dislocations- their types. Colour centers. Solid state reactions - general principles. Experimental procedures. Kinetics of Solid-state reactions (Solid-Solid & Solid-Gas reactions)

(b) Electronic Properties & Band Theory

Free electron theory of metallic solids, Band theory of solids .Semiconductors- Intrinsic & extrinsic semiconductor (n-type & p-type). Doping semiconductors, p-n junction. Super conductors- characteristic properties and applications. Magnetic properties of solids: origin of magnetism in solids, Diamagnetism, paramagnetism – ferromagnetism, antiferromagnetism and ferrimagnetism. Temperature dependence of magnetization.

(c) Catalysis

Pressure difference across curved surfaces (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET equation and its use in estimation of surface area, catalytic

activity at surfaces. Determination of molecular mass of colloidal particles through-Sedimentation, Viscosity and light scattering methods.

Hydrophobic interactions, Micellization, factors affecting the Micellization, Thermodynamics of micellization - phase separation and mass action models, Regular solution theory for mixed micellization

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***Note: Examination Pattern.**

Section-A: Four questions. (Two questions from each unit).

Section-B: Six questions: (Two questions from each unit).

The candidate has to answer any five questions choosing at-least one from each section.