Department of M.Sc. Integrated Chemistry
Palamuru University
Minutes of BoS Meeting

The meeting with all the members of Board of studies was held on the 13th day of January 2025 at 3-5 PM through Zoom virtual meeting mode to finalise the III, IV and V year syllabi for the academic year 2022-23

The meeting was held with following members

SN	Name	Designation
1	**Dr. N. Chandra Kiran**, Associate Professor, Dept. of Chemistry, PU, MBNR	Chairperson
2	**Dr. K. Rajender Reddy**, Chief Scientist, IICT, Hyderabad	Member
3	**Prof. C. Malla Reddy**, Dept. of Chemistry, IIT, Hyderabad	Member
4	**Dr. M. Sridhar Reddy**, Senior Principal Scientist, IICT, Hyderabad	Member
5	**Dr. Md. Noorjahan**, Associate Professor, Dept. of Chemistry, PU, MBNR	Member
6	**Dr. B. Satyanarayana**, Associate Professor, Dept. of Chemistry, JNTU, Hyderabad	Member
7	**Dr. M. Narsingam**, Sr. Scientist, Heterodrugs Pvt Limited, Balnagar, Hyd.	Member
8	**Dr. S. Vijaya Laxmi**, Assistant Professor, Dept. of Chemistry, PU, MBNR	Member
9	**Ms. Afreen Saleha**, Lecturer, TTWRDC, Jedcherla, MBNR	Member
10	**Head**, Dept. of Integrated Chemistry, Palamuru University, MBNR	Member

During the meeting the members suggested various important inputs to further improve the syllabi. After the meeting following resolutions were made and are unanimously approved.

1. Adaptation of Nizam's college syllabi, which was approved in their BoS, from the academic year 2022-23.
2. First 02 years of the program is as per the regular UG curriculum while the last 03 years is as per regular PG curriculum.
3. Seminar presentations are considered as workload, external examinations and accordingly workload is distributed among the faculty.
4. Allotment of department faculty, who has the essential qualifications to become a research supervisor (with a PhD degree and 02 publications post PhD), to supervise the X-sem students of the department for their project dissertations only. Two students are allotted for each faculty.
5. As per the suggestions made by BoS members, few modifications to the Nizam's college syllabus are made and are incorporated in Annexure-I.
6. The proposed syllabi, with modifications, is unanimously approved by the members

Dr N Chandra Kiran
(BoS Chairperson)

(Dr K. Rajender Reddy)

(Prof. C. Malla Reddy)

(Dr. M. Sridhar Reddy)

(Dr Md. Noorjahan)

(Dr. B. Satyanarayana)

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Head, Dept. of. Integ. Chem.

Board of Studies (BoS) Virtual Meeting

On

THE 13th DAY OF JANUARY 2025, at 3-5 PM

Suggestions and Modifications done:

SN	Suggestion Made by members	Modification
1	Syllabus pattern should be uniform to all papers	It is made uniform to all the papers
2	In organic chemistry deletion of topic S-block elements from syllabus	It is deleted from the syllabus While rest of the syllabus (organic, physical and general Chemistry) is taken as it as from Nizam's college
3	To include different salts to be analysed qualitatively in the practicum paper	They are included in the syllabus.
4	To send entire syllabus copy of Nizam's college	It is sent to all the members of BoS

DEPARTMENT OF M.Sc. 5 Yr. INTEGRATED CHEMISTRY (ICY)
PALAMURU UNIVERSITY, MAHBUBNAGAR 509001

PALAMURU UNIVERSITY
M.Sc. Integrated Course in Chemistry
CBCS with effect from Academic year 2022-23 onwards

Semester V

Course Code & Type	Courses	Hours per week	Duration of Exam Hrs.	Marks			No. of Credits
				Internal	External	Total	
ICY-501 (SEC-III)	Basic Computer Skills	2	2	10	40	50	2
ICY-502	Inorganic Chemistry -1	4	3	20	80	100	4
ICY-503	Organic Chemistry -1	4	3	20	80	100	4
ICY-504	Physical Chemistry -1	4	3	20	80	100	4
ICY-505	General Chemistry -1	4	3	20	80	100	4
ICY-551	Inorganic Chemistry -1 (Practical)	6	4		50	50	2
ICY-552	Organic Chemistry -1 (Practical)	6	4		50	50	2
ICY-553	Physical Chemistry -1 (Practical)	6	4		50	50	2
	Seminar	2			25	25	1
	Total	38				**625**	**25**

(Note: Except Skill Enhancement Course (SEC) Remaining Are Core Courses)

Semester VI

Course Code & Type	Courses	Hours per week	Duration of Exam Hrs.	Marks			No. of Credits
				Internal	External	Total	
ICY-601 (SEC-III)	Drug Discovery	2	2	10	40	50	2
ICY-602	Inorganic Chemistry -2	4	3	20	80	100	4
ICY-603	Organic Chemistry -2	4	3	20	80	100	4
ICY-604	Physical Chemistry -2	4	3	20	80	100	4
ICY-605	General Chemistry -2	4	3	20	80	100	4
ICY-651	Inorganic Chemistry -2 (Practical)	4	4		50	50	2
ICY-652	Organic Chemistry -2 (Practical)	4	4		50	50	2
ICY-653	Physical Chemistry -2 (Practical)	4	4		50	50	2
ICY-654	General Chemistry (Practical)	4	4		50	50	2
	Seminar	2			25	25	1
	Total	36				**675**	**27**

(Note: Except Skill Enhancement Course (SEC) Remaining Are Core Courses)

PALAMURU UNIVERSITY
M.Sc. Integrated Course in Chemistry

Semester VII

Course Code & Type	Courses	Hours per week	Duration of Exam Hrs.	Marks			No. of Credits
				Internal	External	Total	
ICY-701 (SEC-III)	Chemistry of Drugs and Pharmaceuticals (705)	2	2	10	40	50	2
ICY-702	Inorganic Chemistry -3	4	3	20	80	100	4
ICY-703	Organic Chemistry -3	4	3	20	80	100	4
ICY-704	Physical Chemistry -3	4	3	20	80	100	4
ICY-705	General Chemistry -3	4	3	20	80	100	4
ICY-751	Inorganic Chemistry -3 (Practical)	4	4		50	50	2
ICY-752	Organic Chemistry -3 (Practical)	4	4		50	50	2
ICY-753	Physical Chemistry -3 (Practical)	4	4		50	50	2
ICY-754	General Chemistry-3 (Practical)	4	4		50	50	2
	Seminar	2			25	25	1
Total		36				675	27

(Note: Except Skill Enhancement Course (SEC) Remaining Are Core Courses)

Semester VIII

Course Code & Type	Courses	Hours per week	Duration of Exam Hrs.	Marks			No. of Credits
				Internal	External	Total	
ICY-801 (SEC)	Intellectual Property Rights	2	2	10	40	50	2
ICY-802	Inorganic Chemistry -4	4	3	20	80	100	4
ICY-803	Organic Chemistry -4	4	3	20	80	100	4
ICY-804	Physical Chemistry -4	4	3	20	80	100	4
ICY-805	General Chemistry -4	4	3	20	80	100	4
ICY-851	Inorganic Chemistry -4 (Practical)	4	4		50	50	2
ICY-852	Organic Chemistry -4 (Practical)	4	4		50	50	2
ICY-853	Physical Chemistry -4 (Practical)	4	4		50	50	2
ICY-854	General Chemistry-4 (Practical)	4	4		50	50	2
	Seminar	2			25	25	1
Total		36				675	27

(Note: Except Skill Enhancement Course (SEC) Remaining Are Core Courses)

PALAMURU UNIVERSITY
M.Sc. Integrated Course in Chemistry

Semester IX

Course Code & Type	Courses	Hours per week	Duration of Exam Hrs.	Marks			No. of Credits
				Internal	External	Total	
ICY-901 (SEC)	Research Methodology	2	2	10	40	50	2
ICY-902	Inorganic Chemistry -5	4	3	20	80	100	4
ICY-903	Organic Chemistry -5	4	3	20	80	100	4
ICY-904	Physical Chemistry -5	4	3	20	80	100	4
ICY-905	General Chemistry -5	4	3	20	80	100	4
ICY-951	Inorganic Chemistry -5 (Practical)	4	4		50	50	2
ICY-952	Organic Chemistry -5 (Practical)	4	4		50	50	2
ICY-953	Physical Chemistry -5 (Practical)	4	4		50	50	2
ICY-954	General Chemistry-5 (Practical)	4	4		50	50	2
	Seminar	2			25	25	1
	Total	36				**675**	**27**

(Note: Except Skill Enhancement Course (SEC) Remaining Are Core Courses)

Semester X

Course Type/ code	Subject	Maximum marks	No. of Credits
Project work ICY-1001	Bench work	250	9
	Project Dissertation	150	8
	Project Seminar	100	4
	Project Viva	100	4
	Total	**600**	**25**

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(BoS Chairperson)

(Prof. C. Malla Reddy)

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Head Dept. of Integrated Chemistry

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-V
Paper I (ICY-501): Skill Enhancement Course (SEC-III)
Basic Computer Skills

Teaching hours-2/week **Credits 2**

Unit I: Introduction to Computers & Fundamentals of an operating system: **8 h**

Introduction to computers: History of computers, Block diagram of a computer – CPU –memory-ROM, RAM, Input / Output Devices.

Operating System: Introduction. What is an OS? Types of OS, OS concepts, Structure of OS, Functions of OS.

Unit II: Introduction to UNIX operating System **6 h**

Introduction to UNIX operating System: Salient features of UNIX – UNIX system organizations, UNIX commands. UNIX system organizations – Types of Shells – sh, ksh, rsh, csh – UNIX commands.

Unit III: Introduction to C Programming Language: **8 h**

Introduction to C Programming Language- Historical development, what is c, where c stands for C preprocessor, features of C preprocessor.

C Programming Language concepts- character set, variables and constants, data types, Arithmetic, relational and logical operators and their hierarchy and associativity – expression and statements. Control statements – if-else and else-if. Switch. Loops – while, for, do-while.

Unit IV: HTML **8 h**

Introduction to HTML - HTML elements – tags and attributes - head, base, meta, title, script and styles – body of HTML – paragraph div, hr, br.

Lists: UL and OL. Nested lists, Images – Types of format – inserting images – attributes.

Tables: table rows, table data, cell and its attributes – table attributes – column span, row span, Style sheets, Hypertext anchors – links to objects.

Suggested Books:

1. Computer Organization and Architecture – Williams Stallings.
2. Operating System – Modern Operating System – Andrew.S. Tenenbaum.
3. UNIX- Shell Programming in UNIX - Yashwant Kanitker.
4. Programming with C – E. Blalaguruswamy (TMH)
5. Programming Using C Language – Byron Gottfried, McGraw Hill (Schaum's series)
6. HTML black book – Steven Holzner.

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-V
Paper II (ICY-502): INORGANIC CHEMISTRY-I

Teaching hours-4/week **Credits 4**

Unit I: Symmetry of molecules
Unit II: Bonding in Metal Complexes-I
Unit III: Coordination equilibria
Unit IV: Ligational aspects of diatomic molecules

Unit I: Symmetry of Molecules: **15 h**

Concept of Symmetry in Chemistry – Symmetry Operations – Symmetry Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry , Inversion Center and Identity Element – More about Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification Molecules in to C_1, C_s, C_i, C_n,C_{nv}, C_{nh}, $C_{\infty v}$, D_n, D_{nh}, D_{nd}, $D_{\infty h}$, S_n (n=even), T_d, O_h, I_h, K_h Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipole moment – Symmetry criteria for Optical activity.

Unit II: Bonding in metal complexes–I: **15 h**

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular Octahedral, tetragonally distorted octahedral, Jahn-Tellar theorem , trigonalbipyramidal, trigonal planar, Pentagonal bipyramidal, and linear geometries. Concept of weak field and strong fields. - Calculation of crystal field stabilization energies (CFSE's) in six and four coordinatecomplexes.Types of magnetic behaviour – magnetic susceptibility – calculation of magnetic moment from magnetic susceptibility spin only formula ,- Quenching of orbital angular momentum – Determination of magnetic moment from Guoy's method.. Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry. Spin crossover: High spin, low spin cross over phenomenon in $[Fe(Ophen)_2(NCS)_2]$ and $[Fe(R_2NCS_2)_3]$. Spinels.

Unit III:CoordinationEquilibria: **15 h**

Solvation of metal ions- Metal complex formation in solution-Binary metal complexes. Stability constants (types and relationships between them). – Factors influencing the stability constants: (i) Metal ion effects (charge/size, IP, crystal field effect, John-Teller effect, Pearson theory of hard and soft acids and bases (HSAB), elecronegativity and hardness and softness, symbiosis. (ii) Ligand effects (Basicity , Substituent effect, Steric , Chelate(size and number of chelate rings), Macrocyclic andCryptate effects- crown ethers, crypton, size match selectivity or concept of hole size, limitations, Macrocycles with pendent groups– Methods used for the determination of Stability constants (Basic Principles only): pH metric, Spectrophotometric and

Polarographicmethods.Ternary Metal Complexes – definition – Formation of ternary metal complexes – Step-wise and simultaneous equilibria with simple examples.

Unit IV: Ligational Aspects of Diatomic molecules **15 h**

Metal Carbonyls:- Carbon monoxide as a ligand – Molecular orbitals of CO - Donor and Acceptor molecular orbitals of CO; Bonding modes of CO- Terminal and Bridging; Evidence for multiple bonding from Bond lengths and Stretching frequencies; 18 Valence electron rule and itsapplication.

Metal Nitrosyls: - NO as a ligand – Molecular orbitals of NO – Donor and Acceptor components; Bonding modes of NO – Terminal (Linear, Bent) and Bridging; Structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and$[RuCl(PPh_3)_2(NO)_2]^+$.
Stereo chemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.
Metal Dinitrogen complexes: - N_2 as aligand – Molecular orbitals of N_2; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru (II) and Os (II) dinitrogen complexes; Chemical fixation of dinitrogen.

Suggested References:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
2. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley &Son(1998).
3. Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Limited(1999).
4. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y(1999
5. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications(1993).
6. Homogeneous Catalysis by Metal complexes Vol I, M MTaqui Khan and A E Martell, Academic Press NY(1974).
7. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-V
Paper III (ICY-503): ORGANIC CHEMISTRY-I

Teaching hours-4/week **Credits 4**

Unit I: Stereochemistry
Unit II: Reaction mechanism-1
Unit III: Conformational analysis (Acyclic systems)
Unit IV: Heterocyclic compounds & Natural products

Unit I:Stereochemistry **15 h**

Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (Cn&Sn). Criteria for Chirality. Desymmetrization.

Axial, planar and helical chirality: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism, planar chiral ansa compounds and trans- cyclooctene, helically chiral compounds and their configurational nomenclature
Relative and absolute configuration: Determination of configuration by chemical correlation methods.

Racemization and resolution techniques: Racemization, resolutions by direct crystallization, diastereoisomer salt formation. Chiral chromatography and asymmetric transformation.

Determination of configuration in E, Z-isomers: Spectral and Chemical methods of configuration determination of E,Z isomers. Determination of configuration in aldoximes and ketoximes.

Unit II:Reaction mechanism-I **15 h**

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond; *anti* addition- Bromination and epoxidation followed by ring opening. *Syn*addition of OsO_4 and $KMnO_4$.

Elimination reactions Elimination reactions E2, E1, E1CB mechanisms. Orientation and stereoselectivity in E2 eliminations. Pyrolytic*syn*elimination and α-elimination, elimination Vs substitution.
Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping and crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

Unit III: Conformational analysis(acyclicsystems) **15 h**
Conformational isomerism: Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers .Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2, 3-diol amino alcohols and 1,1,2,2-tetrahalobutanes. Klyne-Prelog terminology for conformers and torsionangles

Conformations of unsaturated acyclic compounds: Propylene, 1-Butene, Acetaldehyde Propionaldehyde and Butanone.

Factors affecting the conformational stability and conformational equilibrium:
Attractive and repulsive interactions. Use of Physical and Spectral methods in conformational analysis.

Conformational affects on the stability and reactivity of acyclic diastereoisomers: Steric and stereoelectronic factors-examples.Conformation and reactivity. The Winstein-Holness equation and the Curtin – Hammett principle

Unit IV: Heterocyclic compounds&Naturalproducts **15 h**

Heterocyclic compounds: Introduction, Nomenclature, Synthesis and reactivity of indole, quinoline, isoquinoline, carbazole and acridine.
Natural products :Importance of natural products as drugs.
Terpenoids: General methods in the structure determination of terpenes. Isoprene rule. Structure determination and synthesis of β-carotene, α-terpeniolandcamphor.
Alkaloids: General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine

References:

1. Stereochemistry of carbon compounds by Ernest L.Eliel and Samuel H.Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D.Nasipuri
3.Heterocyclic Chemistry, T.L. Gilchrist, Longman UK Ltd, London (1985).
4.Benzofurans A. Mustafa, Wiley-Interscience, New York(1974).
5.HeterocyclicChemistry,3rd EdnJ.A.Joule, K.Mills and G..F.Smith, Stanley ThornesLtd,UK, (1998)
6.The Chemistry of Indole, R.J. Sunderberg, Academic Press, New York(1970).
7.An introduction to the chemistry of heterocyclic compounds, 2ndEdn.R.M.Acheson, Interscience Publishers, New York, 1967.
8.Advanced Organic Chemistry by JerryMarch
9.Mechanism and Structure in Organic Chemistry S.Mukerjee

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-V
Paper IV (ICY-504): PHYSICAL CHEMISTRY -I
Teaching hours-4/week **Credits 4**

Unit I: Thermodynamics-I
Unit II: Electrochemistry-I
Unit III: Quantum Chemistry-I
Unit IV: Chemical Kinetics-I

Unit I: Thermodynamics-I **15 h**

Brief review of I and II Laws of thermodynamics. Concept of Entropy, Entropy as a function of V and T, Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality. Entropy change as criterion for spontaneity and equilibrium. Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Thermodynamic relations. Gibbs equations. Maxwell relations. Gibbs equations for non-equilibrium systems. Material equilibrium. Phase

equilibium. Clausius-Clapeyron equation Conditions for equilibrium in a closed system. Chemical potential of ideal gases. Ideal-gas reaction equlibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

Unit II:Electrochemistry-I **15 h**

Electrochemical Cells: Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination. Types of electrodes. Applications of EMF measurements: Solubility product, potentiometric titrations, determination of pH using glass electrode, equilibrium constant measurements. Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential. 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. Extended Debye-Huckel law. Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations. Concept of ion association – Bjerrum theory of ion association (elementary treatment)-ion association constant – Debye-Huckel-Bjerrum equation.

Unit III: Quantum Chemistry-I **15 h**

A brief review of Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required), Wave particle duality and uncertain principle-significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrödinger wave equation. Operators- Operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators ∇ and ∇^2. Eigen functions and eigen values. Degeneracy. Linear combination of eigen functions of an operator. Well behaved functions. Normalized and orthogonal functions. Postulates of quantum mechanics: Physical interpretation of wave function. Observables and Operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation. Theorems of quantum mechanics. Real nature of the eigen values of a Hermitian operator- significance. Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigen values. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle. Particle in a box- one dimensional and three dimensional. Plots of Ψ and Ψ^2-discussion. Degeneracy of energy levels. Calculations using wave functions of the particle in a box- orthoganality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

Unit IV: Chemical Kinetics- I **15 h**

Theories of reaction rates: Collision theory, steric factor. Transition state theory. Thermodynamic formulation of transition state theory. Application to reaction between atoms and molecules. Limitations of transition state theory. Potential energy surface diagram, Reaction coordinate, Activated complex. Activation parameters and their significance. The Eyring equation. Unimolecular reactions and Lindamann's theory. Complex reactions- Opposing reactions, parallel

reactions and consecutive reactions (all first order type). Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law. Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples. Deviations from Hammett correlations, reasons-Change of mechanism, resonance interaction. Taft four parameter equation. Correlations for nucleophilic reactions. The Swain – Scott equation and the Edward equation. Reactions in solutions: Primary and secondary salt effects. The reactivity-selectivity principle – Isokinetic temperature -Isoselectivty rule, Intrinsic barrier and Hammond's postulate.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press.

2. Physical Chemistry, Ira N. Levine, McGraw Hill.

3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt. Ltd.

4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books.

5. Quantum Chemistry, Ira N. Levine, Prentice Hall.

6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.

7. Chemical Kinetics, K.J. Laidler, McGraw Hill.

8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.

9. Introduction to Electrochemistry, S. Glasstone.

10. Modern Electrochemistry, J. O. M. Bockris& A. K. N. Reddy, Plenum.

11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford& IBH.

12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press. (New York)

13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill.

14. Physical Organic Chemistry, N. S. Isaacs, ELBS.

15. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.

16. Quantum Chemistry – D.A. Mcquarri Viva Publications.

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-V

Paper V (ICY-505): ANALYTICAL TECHNIQUES AND SPECTROSCOPY- I

Teaching hours-4/week **Credits 4**

Unit I: Techniques of Chromatography
Unit II: NMR spectroscopy-I (^{1}H NMR)
Unit III: Rotational and Vibrational spectroscopy
Unit IV: Electronic spectroscopy

Unit I: Techniques of Chromatography **15 h**

i. Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory.
ii. GC: Principle, instrumentation, detectors- TCD, FID, ECD. Derivatization techniques, PTGC.
iii. HPLC: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.
iv. Applications: Methods of quantization for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assay of paracetamol and aspirin in tablets.

Unit II: NMR spectroscopy-I (^{1}H-NMR) **15 h**

^{1}H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ^{1}H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging (MRI). ^{1}H NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, asprin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ (Rh I=1/2), $[Pt(acac)_2]$.

Unit III: Rotational, Vibrational and Raman spectroscopy **15 h**

a) Microwave Spectroscopy: Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief

description of microwave spectrometer.

b) Vibrational Spectroscopy. Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation force constant from vibrational frequency. Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi Resonance. Vibration rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency. IR spectra of metal coordinated NO_3^-, SO_4^{2-} and CO_3^{2-}ions.

c) Raman Spectroscopy- Classical and Quantum theories of Raman effect. Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

Unit IV: Electronic spectroscopy **15 h**

Electronic spectroscopy**:** Electronic spectra: Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Congugated dienes, trienes and polyenes, unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di substituted derivative (R-C_6H_4-R′) and substituted benzene derivatives (R-C_6H_4-COR′), Woodward-Fieser rules. Polynuclear aromatic compounds (Biphenyl, stilbene, naphthalene, anthracene, phenanthrene and pyrene). Heterocyclic systems. Absorption spectra of charge transfer complexes. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation. Beer's law application to mixture analysis and dissociation constant of a weakacid.

References:

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M.Barrow.
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp.
9. Atomic Structure and Chemical bond: including Molecular Spectrodcopy, Manas Chanda,
10. Spectroscopy of organic compounds, P.S. Kalsi.
11. Structural methods in Inorganic chemistry, E.A.V Ebsworth.
12. Organic Spectroscopy, LDS Yadav
13. Organic Spectroscopy, Y.R.Sharma
14. Molecular Spectroscopy –Arhuldas
15. Vibrational spectroscopy – D.N. Satyanaraya

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practical
Paper VI (ICY-551): Inorganic Chemistry- I

Teaching hours-4/week Credits 2

I. Calibrations:
(i) Calibration ofweights.
(ii) Calibration ofpipettes.
(iii) Calibration of standardflasks.
(iv) Calibration ofburette.
II. EDTAback-titrations:
(i) Estimation ofNi^{2+}.
(ii) Estimation ofAl^{3+}.
III. EDTA substitutiontitrations:
Estimation of Ca^{2+}.
IV. RedoxTitrations
(i) Estimation of Ferrocyanide and Ferricyanide in a mixture
V. Preparation ofcomplexes:
(i). Hexaammine nickel (II) chloride.
(ii). Tris (acetylacetanato) manganese.
(iii). Tris (ethylenediamine) nickel (II) thiosulphate.
(iv). Mercury tetrathiocyanatocobaltate (II).
(v). Chloropentaammine cobalt (III)chloride
(vi). Tetrammine copper (II) sulphate and estimation of NH_3 and calculation of %purity.

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Paper VII (ICY-552): Organic Chemistry -I

Teaching hours-4/week Credits 2

Synthesis of the following compounds:
p-Bromoacetanilide,
p- Bromoaniline,
2,4,6- tribromoaniline,
1,3,5-tribromobenzene,
aspirin,
tetrahydrocarbazole,
7-hydroxy-4-methyl coumarin,
m-dinitrobenzene,
m-nitro aniline,

hippuric acid,
azalactone,
anthracene-maleic anhydride adducts,
Phthalimide,
2,4-dihydroxyacetophenone

References.

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.

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Practical

Paper VIII (ICY-553): Physical Chemistry - I

Teaching hours-4/week Credits 2

A. Chemical Kinetics:

1. Stoichiometry of $K_2S_2O_8$ –KI reaction

2. Overall order of $K_2S_2O_8$ –KI reaction

3. Order with respect to $K_2S_2O_8$ using initial rate method
4. Order with respect to KI using initial rate method

B. Distribution:

5. Distribution of Iodine between n–hexane and water

6. Distribution of Iodine between n–hexane and aq. KI (Calculate equilibrium constant)

7. Distribution of succinic acid between water and ether

C. Polarimetry:

8. Determination of specific rotation of Sucrose, Glucose and Fructose

9. Acid catalyzed hydrolysis of Sucrose (Inversion of Sucrose)

10. Enzyme catalyzed hydrolysis of sucrose

D. pH-metry:

11. Calibration of a pH meter and measurement of pH of different solutions

12. Preparation of phosphate buffers

13. Titration of strong acid vs strong base

14

E. CST:

14. Determination of CST of of phenol-water system

15. Effect of added electrolyte on the CST of phenol-water system

References:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.

2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, AdarshGulati

3. Experimental Physical Chemistry: V. Athawale and P. Mathur.

4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.

5. Practical in Physical Chemistry: P.S. Sindhu

6. Advanced Practical Physical chemistry: J.B.Yadav

PALAMURU UNIVERSITY
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SEMESTER-VI

Paper I (ICY-601): Skill Enhancement Skill Course (SEC-IV)
Computational Chemistry and Drug Designing

Teaching hours-2/week **Credits 2**

Unit I: Computational Chemistry

Unit II: Drug Designing

Unit I: Computational Chemistry **15 h**

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems, Cartesian and internal Coordinates, Z-matrix, Potential energy surface - Conformational search - Global minimum, Local minima, Conformational analysis of ethane. Force field - Features of Molecular Mechanics –Bonded and Non-bonded interactions. Bond Stretching – Angle Bending, Torsional Terms – Improper Torsions and out of Plane Bending Motions – Cross Terms. Non Bonded Interactions – Electrostatic Interactions - Van-der Waals interactions - Hydrogen Bonding, Miscellaneous interactions. Force Field Equation in Energy minimization (Energy as function of r, ɵ, ω) and variation w.r.t ω only - Introduction to Derivative Minimization Methods – First Order Minimization – The steepest Descent Method – Conjugate Gradients Minimization – Conformational Search procedures - Geometry optimization procedures - Introduction to molecular dynamics.

Unit II: Drug Designing **15 h**

Ligand Based

Lead Molecule - Structure Activity Relationship (SAR) –QSAR- Physicochemical parameters, Hydrophobicity, Electronic effects, Steric Factors: Molar refractivity, Verloop steric factor and other physicochemical parameters. Methods used in QSAR studies- Correlation of Biological activity with physico chemical Parameters – Application of Hammet equation, Hansch analysis, significance of slopes and intercepts in Hansch analysis. QSAR- 2D Linear Free Energy Relationship (LFER) - Craig plot - Topliss scheme - Bioisosteres - Free- Wilson approach - Molecular Descriptor analysis - Structure representation.

Structure Based.

Homology Modeling – Model Evaluation: Ramachandran Plot - Active site Identification - Docking - Docking Algorithms- Interactions-Scoring-Virtual Screening - Small molecule Building – De novo ligand design.

References:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.

2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.

3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.

4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003

5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996

6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition.

7. Bioinformatics – A Primer by P. Narayanan, New Age International, (P) Ltd, 2005.

8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002

9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007

10. Principles of Medicinal Chemistry, by Patrick

11. Bioinformatics: Methods : Genomics, Proteomics and Drug Discovery. S.C. Rastog,NamitaMendiratta, Parag Rastogi, PHI Larning Pvt.Ltd; 2006

12. Pharmacy Practice Vol.I and II by Remington.

13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition

14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- larsen tommy liljefors and ULF madsen.

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Paper II (ICY-602) INORGANIC CHEMISTRY-II

Teaching hours-4/week **Credits 4**

Unit V: Reaction mechanisms of transition metalcomplexes
Unit VI: Bonding in metal complexes-II
Unit VII: Metal clusters
Unit VIII: Biocoordination chemistry

Unit V: Reaction mechanisms of transitionmetalcomplexes: **15 h**

Ligand substitution reactions:
Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE, SN, SN^1, SN^2). Langford and Grey classification – A mechanism, D-Mechanism, I_a, I_d, and Intimate mechanism.
Ligand substitution reactions in octahedral complexes:
Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis , Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN^1CB Mechanism.
Substitution reactions without Breaking Metal-Ligand bond. Anation reaction
Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Trans-influence, Grienberg's Polarization theory and Π - bonding theory – Applications of Trans-effect in synthesis of Pt (II) complexes.
Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds: Mechanism of One-electron Transfer Reactions: Atom (or group) Transfer or Inner Sphere Mechanism, Direct electron Transfer or Outer Sphere Mechanism. Factors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

Unit VI: Bonding in Metal Complexes–II: **15 h**

Free ion terms and Energy levels: Configurations, Terms, States and Microstates – Formula for the calculation of Microstates p^n and d^n configurations – L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various p^n and d^n configurations of metal ions. Hole formalism – Energy ordering of terms (Hund's rules) Inter – electron repulsion Parameters (Racah parameters) – Spin-Orbital coupling parameters. Effect of weak cubic crystal fields on S,P,D and F terms- Orgel Diagrams.

Unit VII: MetalClusters: **15 h**

Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters – Low Nuclearity Clusters : M_3 and M_4 clusters , structural patterns in $M_3(CO)_{12}$ (M=Fe,Ru,Os) and $M_4(CO)_{12}$ (M=Co,Rh,Ir) Clusters. Metal carbonyl scrambling – High Nuclearity clusters M_5, M_6, M_7, M_8 and M_{10} Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Capping rule – Structural patterns in $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $\{Os_7(CO)_{21}\}$, $\{Rh_7(CO)_{16}\}^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$.

Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and trigonal antiprismatic structures -. Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications. Boranes, carboranes, STYX Rule. Stereo chemical non-rigidity in $[Rh_4(CO)_{12}]$ and $[Fe_2(Cp)_2(CO)_4]$.

Unit VIII: Bio-coordination chemistry: **15 h**

Metal ions in Biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements.

Oxygen transport and storage: Hemoglobin (Hb) and Myoglobin (Mb) primary, secondary, tertiary and quarternary structures and non-covalent bonds present in them. Oxygenation equilibria for Mb and Hb. Factors effecting oxygenation equilibria. Cooperativity and its mechanism. Spin state of iron. Spatial and electronic aspects of dioxygen binding. Allosteric models (T and R states). Role of globin. Transport of NO and CO_2. Hemocynin (Hc) and Hemerythrin (Hr): Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II. Vitamin B_6 model systems: Forms of vitamin B_6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions.

References:

1. Inorganic Reaction Mechanisms. M.L.Tobe and John Burgess, Addison Wesley Longman (1999).
2. Metal ions in Reaction Mechanisms. K.Veera Reddy. Golgotia Publications (P)Ltd
3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London(1993).
4. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York(1967).
5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 Th Edition, Wiley Interscience, N.Y(1999
6. Inorganic Chemistry, J.E.Huheey ,K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications(1993).
7. Inorganic Biochemistry Edited by G.L.Eichorn, Volume 1 Elsevier (1982).
8. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY(1990).
9. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London(1977).
10. Bioinorganic Chemistry, I.Bertini, H.B.Gray, S.J. Lippard and S.J. Valentine, Viva Low-Priced Student Edition, New Delhi(1998).
11. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W. Kaim and B.Schwederski, John Wiley and Sons, NY(1999).

PALAMURU UNIVERSITY
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SEMESTER-VI

Paper III (ICY-603) ORGANIC CHEMISTRY-II

Teaching hours-4/week **Credits 4**

Unit V: Reaction mechanism-II
Unit VI: Pericyclic reactions-I
Unit VII: Photochemistry
Unit VIII: Reactive intermediates and molecular rearrangements

Unit V:Reaction mechanism-II **15 h**

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: $S_N1(Ar)$, S_N2 (Ar), and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles.

Neighbouring group participation : Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighbouring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalky l groups , σ and π- bonds. Introduction to nonclassicalcarbocations. Electrophilic substitution at saturated carbon and single electron transfer reactions.

Mechanism of aliphatic electrophilic sustitution. S_E1, S_E2, and S_Ei. SET mechanism.

Unit VI: Pericyclic reactions **15 h**

Introduction, Classification of pericyclic reactions,

Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems.

Cycloaddition reactions: suprafacial and antara facial additions in 4n and 4n+2 cycloadditions.

Sigmatropic reactions: [i, j] shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.

Approaches for the interpretation of mechanism of pericyclic reactions: Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel

–Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allylcation, allyl radical, pentadienylcation, pentadienyl radical.

Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry: (Correlation Diagrams) approach- for electrocylic and cycloadditions &cycloreversions.

Unit VII: Photochemistry **15 h**

Photochemistry: Photochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene Electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimeriastion of simple and conjugated olefins. Addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene.
Photochemistry of (n-π*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α-bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.
Intermolecular abstraction of hydrogen: photoreduction-influence of temperature, solvent, nature of hydrogen donor and structure of the substrate.
Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction,
Photochemistry of nitrites-Barton reaction.

Unit VIII: Reactive intermediates and Molecular rearrangements **15 h**

Reactive Intermediates: Generation, detection, structure, stability and reactions ofcarbocations, carbanions, carbenes, nitrenes and free radicals.
Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalyzed rearrangements: Benzilic acid, Favourski, Transannular, Sommlett-Hauser and Smiles rearrangement

References :

1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H.Wilen
2. Stereochemistry of organic compounds – Principles and Applications by DNasipuri
3. The third dimension in organic chemistry, by AlanBassindale
4. Stereochemistry: Conformation and Mechanism by P SKalsi
5. Stereochemistry by V MPotapov
6. Advanced Organic Chemistry by JerryMarch
7. Mechanism and Structure in Organic Chemistry S.Mukerjee
8. Organic chemistry Vol.I and II byI.L.Finar
9. Comprehensive organic chemistry Vol.5 D.H.R.Barton andW.D..Ollis

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Paper IV (ICY-604) PHYSICAL CHEMISTRY-II

Teaching hours-4/week **Credits 4**

Unit V: Thermodynamics-II & Statistical Thermodynamics
Unit VI: Photochemistry-I
Unit VII: Quantum Chemistry-II
Unit VIII: Solid state chemistry

Unit V: Thermodynamics-II & Statistical Thermodynamics **15 h**

Partial molar poperties-significance. Relation between solution volume and partial molar volume. Measurement of partial molar volumes- slope and intercept methods. The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance.

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. Nonideal systems. Concept of fugacity, fugacity coefficeient. 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 nonvolatile solutes using Gibbs-Duhem equation. Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

Unit VI: Photochemistry–I **15 h**

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules-singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield and its determination. Experimental set up of a photochemical reaction. Actinometry-ferrioxalate and uranyl oxalate actinometers – problems. Derivation of fluorescence and phosphorescence quantum yields. E-type & P-type delayed fluorescence- evaluation of triplet energy splitting (ΔE_{ST}). Photophysical processes- photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams Photochemical primary processes. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern-Volmer equation. Introduction to fast reactions-Principle of flash photolysis. Formation of excimers and exciplexes- their quantum yields

Unit VII: Quantumchemistry-II **15 h**

Cartesian, Polar and spherical polar coordinates and their interrelations.
Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and theirimportance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour pots and boundary diagrams.
Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Paricle in a box.

Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant.

Bonding in molecules: Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variationan integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

Unit VIII: Solid state chemistry **15 h**

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors. Photo conductivity and photovoltaic effect – p-n junctions.

Superconductivity: Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner effect. Types of superconductors. Theories of super conductivity – BCS theory. High temperature superconductors: Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$. Prepartion of 1-2-3 materials. Origin of high T_c superconductivity.

Classification of solids based on magnetic properties: Paramagnetic, Diamagnetic, Ferro, antiferro, Langvien theory of diamagnetic materials.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press.
2. Physical Chemistry, Ira N. Levine, McGraw Hill.
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, VivaBooks Pvt Ltd.
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books.
5. Quantum Chemistry, Ira N. Levine, Prentice Hall.
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill.
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International.
9. Solid state Chemistry and its aplications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern.
11. Molecular Photochemistry, N.J. Turro, Benjamin.
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson.
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell, Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.

15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

16. Principles of the Solid State, H. V. Keer, New Age International.

17. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.

18. Quantum Chemistry, D.A. McQuarrie, Prentice Hall.

19. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.

20. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press.

21. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum.

22. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.

23. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.

24. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

25. Solid State Chemistry, Gurtu-Gurtu, PragatiPrakashan, Meerut.

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SEMESTER-VI

Paper V (ICY-605) ANALYTICAL TECHNIQUES and SPECTROSCOPY - II

Teaching hours-4/week **Credits 4**

Unit V: Electro analytical Techniques.
Unit VI: NMR- II
Unit VII: Mass Spectroscopy
Unit VIII: Photoelectron & ESR spectroscopy

Unit V: Electro Analytical Techniques 15 h

Types and Classification of Electro analytical Methods:

a) D.C Polarography:. Instrumentation - Dropping mercury electrode- -polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants ofcomplexes.

b) Brief account of following techniques and their advantages over conventional d.c.polargraphy.

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography

c) Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances.

d) Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticideparathion.

Unit VI: NMR spectroscopy-II (^1H, ^{19}F and^{31}PNMR) 15 h

^1H, ^{19}F, ^{31}P and solid state NMR spectroscopy: First order and non first order spectra e.g., AX, AX_2, AX_3, A_2X_3, AMX and AB, ABC. Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid. Nuclear Overhauser enhancement (NOE). Fluxional moleculesbullvalene, [η5-C_5H_5M], [η5-$(C_5H_5)_2$ Ti η1-$(C_5H_5)_2$] and [η4$C_8H_8Ru(CO)_3$].

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F, ^1H and ^{31}P: 1,2 dichloro-1,1 difluoro ethane, BrF_5, SF_4, PF_5, ClF_3, IF_5,CF_3CH_2OH

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P, ^{19}F, ^1H and ^{13}C: ATP, Ph_3PSe, P_4S_3, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH3, $[Rh(PPh_3)Cl_3]$ (Rh I=1/2)

Introduction to solid state NMR: Magic angle spinning (MAS).Applications of solid state NMR.

Unit VII: Mass spectrometry **15 h**

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mclafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

Unit VIII: Photoelectron & ESR spectroscopy **15 h**

Photo electron Spectroscopy: Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2 - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance: Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy and quadrupolar interactions. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalcylaldimine, Bis-acetylacetanatovanadyl(II) and hexachloroiridium(IV) complexes.

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W.J ohnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectroscopic identification of organic compounds by R.M.Silverstein. C.Basslerand T.E. Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.
12. Principles of Polarography, Kapoor.

13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.

14. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.

15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders college Publishing.

16. International series of Monographs, Vol. **53**: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.

17. Sructural methods in inorganic chemistry, E.A.V. Ebsworth

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VI
Practical
Paper VI (ICY-651): Inorganic Chemistry -2

Teaching hours-4/week Credits 2

I Applied titrimetric analysis

(i) Determination of Iron and calcium in Cement
(ii) Determination of Calcium in calcium tablets
(iii)Determination of alkali content in antacid
(iv) Determination of Ca^{2+}, Mg^{2+}, CO_3^{2-} , HCO_3^- in soil sample
(v) Determination of saponification value, Iodine number (5-6 samples and comparative study)
(vi) Determination of residual Chlorine in water by Iodometry.
(vii) Determination of Dissolved Oxygen in water sample

Suggested Books: (For both semesters).

1. (i). Text book of Quantitative Inorganic Analysis by A.I. Vogel, 3rd edition, ELBS 1969. (ii). Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS 1988. (iii). Vogel's text book of Quantitative Inorganic Analysis. 6th edition, Pearson education ltd 2002.
2. Practical Inorganic chemistry By G.Marr and R.W.Rockett1972.
3. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work. By MounirA.Malati,1999.
4. Advanced experimental Inorganic chemistry by. AyodhyaSingh.
5. Practical Inorganic Chemistry by G. Pass & H. Sutchiffe, 2ndedn John Wiley &sons.
6. Comprehensive Experimental Chemistry by V.K. Ahluwalia et.al New Age Publications 1997.
7. Analytical Chemistry-Theory and Practice by R.M. Verma 3rd Ed. CBS Publishers & Distributors 1994

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VI
Practical
Paper VII (ICY-652): Organic Chemistry - 2

Teaching hours-4/week Credits 2

Identification of organic compounds systematic qualitative analysis:

Physical data BP / MP, Ignition test, solubility classification, Extra elements-N,S&

Halogens, (Lassagnine sodium fusion test, Beilstein test)
Functional groups tests, Preparation of crystalline derivative and determination of their m.p.s and reference to literature to identify the compounds
A minimum of **8** following compounds to be studied as unknown covering atleast one from each of the solubility classes
Glucose, benzoic acid, 2-chloro benzoic Acid, Anisic acid, p-Nitrobenzoic acid; p-Cresol, p- Chlorophenol, □-Naphthol; Aniline, o/m/p-Chloroanilines; N-Methyl aniline/N-Ethylaniline, N,N-Dimethylaniline,Benzamide, Benzaldehyde, Anisaldehyde, Acetophenone,benzophenone,Ethylbenzoate,methylbenzoate,Nitrobenzene, chlorobenzene, bromobenzene , naphthalene, biphenyl anthracene.

Identification of unknown organic compounds from their IR, UV, ^{1}H-NMR and MS:
Analysis of recorded spectra of 6 compounds belonging to i) aromatic carboxylic acid ii) alcohols and phenols iii) aldehydes and ketones iv) amides v) esters vi) alkenes and alkynes

References

1. Text book of practical organic chemistry,Vogel
2. Text book of practical organic chemistry, Mann andSaunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5thEdition

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VI
Practical

Paper VIII (ICY-653): Physical Chemistry practical-2

Teaching hours-4/week **Credits 2**

Kinetics and Instrumentation

(A) Chemical Kinetics

$K_2S_2O_8$-KI reaction

1. Order with respect to KI using isolation method
2. Order with respect to $K_2S_2O_8$ using isolation method
3. Effect of Ionic strength on reaction rate
4. Effect of temperature on reaction rate
5. Effect of solvent (Acetonitrile, Methanol and 1,4 dioxane) on reaction rate
6. Effect of Ionic strength on uncatalysed and Cu(II) –catalyzed reactions.

(B) Instrumentation – Conductometry

1. Strong acid vs Strong base
2. Weak acid vs Strong base
3. Mixture of strong and weak acids vs strong base
4. Mixture of strong and weak bases vs strong acid
5. Mixture of strong acid, weak acid and metal ions ($CuSO_4$, $ZnSO_4$, $MgSO_4$, $NiSO_4$) vs strong base
6. Mixture of halides (chloride + iodide) vs $AgNO_3$
7. Precipitation titration: K_2SO_4vs $BaCl_2$
8. Dissociation constants of weak acids
9. Effect of solvent (Acetonitrile, Methanol and 1,4 dioxane) on dissociation constant of acetic acid
10. Verification of Onsager equation for KCl, KBr and KI
11. Composition of Cu(II) – tartaric acid complex by Job's method

References:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1& 2.

2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, AdarshGulati

3. Experimental Physical Chemistry: V. Athawale and P. Mathur.

4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.

5. Practical in Physical Chemistry: P.S. Sindhu

6. Advanced Practical Physical chemistry: J.B.Yadav

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VI
Practical
Paper IX (ICY-654): General Chemistry practical-2

Teaching hours-4/week Credits 2

I One component gravimetric estimations

(i) Estimation of Zn^{2+}
(ii) Estimation of Ba^{2+} (as $BaSO_4$)

II Analysis of Two component mixtures:

(i). Separation of Ni^{2+} and Cu^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+}

(volumetric).

III Analysis of three component mixtures:

(i). Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} (Gravi).

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER VII
PAPER - I (ICY-701) Skill Enhancement Course (SEC-V)

Chemistry of Drugs and Pharmaceuticals — Credits 2

Unit — III: General Characteristics of Drugs — **15 h**

Introduction: Diseases — causes of diseases, Drug — definition and sources.
ADME of drugs (brief) — Absorption, distribution, drug metabolism (in liver), elimination (brief). Toxicity.

Examples (i) Zintac (Ranitidine, antacid) (ii) Paracetamol (antipyretic) (iii) Benadryl (Cough syrup). Characteristics of an ideal drug.

Nomenclature of Drugs: chemical name — generic name — trade name. Trade names for the given generic names — (i) Aspirin (ii) Amoxycillin (iii) Ciprofloxacin (iv) Paracetamol (v) Mebendazole.

Drug formulations: Definition — need for conversion of drug into pharmaceutical (drug formulations) — Additives — diluents, binders, lubricants, antioxidants, flavourants, sweeteners, colourants, coating agents.

Classification of Drug formulations: oral, parenterals and topical dosage forms - advantages and disadvantages.

(i) Oral Dosage forms: Tablets (Aspirin — analgesic; Ciprofloxacin - antibacterial). Capsules (Amoxycillin — antibiotic; Omeprazole-antacid). Syrups (B-complex syrup; Benadryl- Cough syrup).
(ii) Parenterals (Injection forms): Propranolol (antihypertensive), Heparin (anticoagulant)
(iii) Topical dosage forms: Creams and Ointments
(iv) Antiallergic: Aclometasone (Aclovate), Betamethasone valerate(2%) Multiple purposes,
(v) Anti-itching: Doxepin Zonalon), Antifungal: Miconozole (Dactarin, Neomicol), Ketoconazole, (Nizoral Cream), Fluconazole, Anesthetic-Lidocaine, (Lidocaine ointment) and Antiseptic: Boro Plus Cream, For burns-Iodine ointment.

Unit — IV: Classification of Drugs — **15 h**

Classification of drugs based on therapeutic action-Chemotherapeutic agents, Pharmacodynamic agents and drugs acting on metabolic processes.

Brief explanation for the following :

(i) Chemotherapeutic agents: Antimalarials-Chloroquine; Antibiotic-Amoxicillin;

Antitubercular drugs – isoniazide; Antiprotozoals-metronidazole.

(ii) Pharmacodynamic agents :
   a) Drugs acting on CNS: Diazepam (CNS depressant), General anesthetic (Thiopental sodium), antipyretic and analgesic (Iburofen)
   b) Drugs acting on PNS: local anasthetics (Benzocaine)
   c) Drugs acting on cardiovascular system: Metaprolol (antihypertensive agents), Nefidipine antianginal and antihypertensive agent).
   d) Drugs acting on renal system: Diuretics (Acetazolamide).

(iii) Drugs acting on metabolic processes :
   a) Vitamins: Common name, source, deficiency, vitamin A, B2, B6, C, D, E and K – remedy
   b) Hormones: Function (brief) – deficiency of hormones (Insullin, Testosterone and Oesterone).

Recommended Text Books and Reference Books:

1. An Introduction to Medicinal Chemistry by Graham L. Patrick, Oxford University Press, New York,1995.
2. Drugs by G.L. David Krupadanam, D. Vijaya Prasad, K. Varaprasad Rao, K.L.N.Reddy, C. Sudhakar, Universities Press (India) Limited 2007.
3. Introduction to drug design by R Silverman
4. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
5. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
6. Medicinal Chemistry By Ashtoshkar
7. Principles of medicinal chemistry. By William O. Foye.
8. Medicinal chemistry An introduction By Gareth Thomas.

PALAMURU UNIVERSITY
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SEMESTER-VII

PAPER II (ICY-702) INORGANIC CHEMISTRY-III

Teaching hours-4/week **Credits 4**

Bonding Group Theory and its Applications

Unit IX: Group Theory, Normal mode analysis and Spectral Activity
Unit X: MOT of Metal Complexes
UnitXI: Electronic Spectroscopy of Metal Complexes
Unit XII: IR and Raman Spectroscopy

Unit IX: Group Theory, Normal Mode Analysis and Spectral Activity **15 h**

Properties of a Group-Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups. Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, salient features about Classes, Classes of C_{2V}, C_{2h} and C_{3V}. Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of *E, Cn, Sn*, i and σ Elements. Great Orhogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for C2V, C2hand C3V. Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula. Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for IR and Raman activity. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for C_{2V} (eg. H_2O, SF_4), C_{3V} (NH_3, $POCl_3$), C_2h (trans-N_2F_2), D_3h (BF_3), Td(SO_4^{2-}), Oh (SF_6). Internal coordinate method of analysis for C_2V (H_2O), C_3V (NH_3), Td (SO_4^{2-}).

Unit X: Molecular Orbital Theory of Metal Complexes: **15 h**

Limitations of Crystal Field Theory,Adjustments to the Crystal Field Theory to allow for covalence -Experimental evidences for Metal -Ligand orbital overlap. The Adjusted Crystal Field Theory. Introduction to Molecular Orbital Theory.Symmetry Classification of Metal and Ligand Group Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams -Octahedral Metal Complexes with (i) Sigma (σ), (ii) sigma(σ) &Pi (π) and (iii) sigma (σ), Pi (π) and Pi* (π*) bonding contribution from the Ligands - Tetrahedral Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi(π), and Square Planar Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π) bonding contribution from the ligands - Molecular orbital electron configurations and calculation of Magnetic Moments.

Unit XI: Electronic Spectroscopy of Metal Complexes **15 h**

Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for d^1-d^9 Configurations, Crystal Field Spectra of Oh and Td Metal Complexes of 3d Metals. Charge Transfer Spectra. Strong Field Configurations: The Method of Descending Symmetry, Correlation Diagrams and Tanabe-Sugano Diagrams for d^2 and d^8 Configurations. Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β).

Unit XII: Infrared and Raman Spectroscopy **15 h**

Conditions for Infrared and Raman Spectroscopies, Direct product – symmetry requirements for overtones, binary and ternary combination bands. Partial Normal mode analysis-Structure Fitting,

Determination of Coordination Sites and Linkage Isomers(NO_2^- , SCN^-), Assigning Denticity of Ligands (SO_4^{2-}, CO_3^{2-}), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Nitrogen, Carbon and Halogen Donors (NH_3, H_2O, Glycine, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, CO_2, N_2O, H_2O.Principles of Resonance Raman Spectroscopy. Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers.

SUGGESTED BOOKS

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International

(P) Limited Publishers (2009)

2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)

3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)

4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press,

NY (1995)

5. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)

6. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)

7. Molecular Symmetry, Schoenland

8. Electronic Spectroscopy, A. B. P. Lever

9. Introduction to Ligand fields, B. N. Figgis

10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto

11. Infrared spectroscopy of Inorganic Compound, Bellamy.

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VII

PAPER III (ICY-703) ORGANIC CHEMISTRY-III

Teaching hours-4/week **Credits 4**

Synthetic Reagents, Conformational Analysis and ORD, Carbohydrates

Unit-IX: Synthetic Reagents-I
Unit-X: Synthetic Reagents-II
Unit-XI: Conformational analysis (Cyclic systems) & ORD
Unit-XII: Carbohydrates

Unit-IX: Synthetic Reagents-I **15 h**

i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiolacetal (Umpolung)groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organolithium 2) Organo copper reagents3) Organoboranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethylsilyl halides, cyanides and triflates.

iii) Carbonyl methylenation: a) Phosphorousylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction.b) Titanium- Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.

iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.

v) C-H Activation: Introduction, Rh catalysed C-H activation.

Unit-X: Synthetic Reagents II **15 h**

i) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO2.b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls: CrVI oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation)and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications. e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

Unit-XI: Conformational analysis (Cyclic systems) & ORD **15 h**

Conformational analysis (Cyclic systems): Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethylcyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane . Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, NMethylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. (oxidation, SN2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempiricalrules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

Unit-XII: Carbohydrates **15 h**

Introduction to the importance of Carbohydrates. Types of naturally occurring sugars. Deoxy sugars, amino sugars, branched chain sugars methyl ethers and acid derivatives of sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. $^4C_1$ and $^1C_4$ conformations of D-glucose. Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement. Synthesis of amino, halo and thio sugars. Structure, ring size determination of sucrose and maltose. Conformational structures of sucrose, lactose, maltose, cellobiose and gentobiose. Structure and biological functions of starch, cellulose, glycogen and chitin. Role of sugars in cell to cell recognition, blood groups.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers

2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R AAtken

3. Organic Synthesis by O House

4. Organic synthesis by Micheal B Smith

5. Reagents for organic synthesis, by Fieser&Fieser, Vol 1-11 (1984)

6. Organic synthesis by Robert E Ireland

7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV

8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren

9. Organic Reactions and their mechanisms by P.S.Kalsi

10.Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar

22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri

23. Stereochemistry of Carbon compounds by Ernest L Eliel& Samuel H. wilen

24. Stereochemistry: Conformation & Mechanism by P S Kalsi

25. The third dimension in organic chemistry, by Alan Bassendale

26. Stereo selectivity in organic synthesis by R S Ward.

27.Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg

28. Optical rotatory dispersion by C Djerassi

29. Optical rotatory dispersion and circular dichroism by P Crabbe

30. Mechanism and Structure in Organic chemistry by S Mukherjee

31. Organic Chemistry Vol.I and Vol.II by I.L.Finar

32. Carbohydrate Chemistry by Barton Volumes

33. Carbohydrate chemistry by G.J.Boons

34. The chemistry of natural products:vol.V - carbohydrates by S.F.Dyke

35. Organic Chemistry by McMurry

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VII

PAPER IV (ICY-704) PHYSICAL CHEMISTRY-III

Teaching hours-4/week **Credits 4**

Unit-IX: Applications of Schrödinger equation
Unit- X: Chemical kinetics – II
Unit- XI: Electrochemistry – II
Unit- XII: Statistical Thermodynamics

Unit-IX: Applications of Schrödinger equation **15 h**

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3 , hydrogen transfer reactions. The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model. The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule. The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations. Atomic and molecular term symbols. Atoms in external field, Zeeman and anomalous Zeeman effect.

Unit- X: Chemical kinetics – II: 15 h

Reactions in solution: Factors affecting reaction rates in solution. Effect of pressure on rate ofreaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

Unit- XI: Electrochemistry – II **15 h**

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.
Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.
Corrosion: Electrochemical corrosion.Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion.Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

Unit- XII: Statistical Thermodynamics **15 h**

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles. The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy. Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory. The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies. The relation between equilibrium constant and partition function- derivation. Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press
5. Coulson's Valence, R. McWeeny, ELBS
6. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
7.. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
8. Statistical Thermodynamics, M. C. Gupta, New Age International
9. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
10. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
11. Text book of Biochemistry by Stryer, W.H.Freeman & Co Ltd
12. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
13. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
14. Chemical Kinetics, K. J. Laidler, McGraw Hill
15. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
16. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan

17. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
18. Physical Organic Chemistry, N. S. Isaacs, ELBS
19. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
20. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
21. Modern Electrochemistry 2B, Bockris & Reddy, Plenum.
22. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VII

PAPER V (ICY-705) ANALYTICAL TECHNIQUES AND SPECTROSCOPY-III
Teaching hours-4/week **Credits 4**

UNIT-IX : ^{13}C NMR and 2D NMR spectroscopy
UNIT –X : Diffraction Methods
UNIT XI: Thermal Methods
UNIT XII: Advanced Mass spectrometry

UNIT-IX : ^{13}C NMR and 2D NMR spectroscopy **15 h**

i) ^{13}C NMR spectroscopy: Introduction, Types of ^{13}C NMR spectra: undecoupled, proton decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C,^{1}H J and ^{13}C, ^{1}H J) coupling. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}CNMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (1H-1H COSY) , TOCSY (Total Correlation Spectroscopy), HeteroCOSY (^{1}H, ^{13}C COSY,HMQC), long range -^{1}H, ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D INADEQUATE experiments and their applications.

UNIT –X: Diffraction Methods **15 h**

X – ray Diffraction : X –rays and their generation – choice of radiation ; Miller indices, Braggs equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X – rays – Platinum phthalocyanine complex, Silylacetate, Tetraalkylbiphosphate ; Advantages and limitations of X – ray Diffraction.

Electron Diffraction by gases :Principles , Radial distribution curves- Interpretation of results for $PBrF_2S$, PF_3S, PF_2HS, $HClO_4$, Silylmonothioacetate and Germylmonothioacetate and HgCl2 molecules, Advantages and Limitations.

Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies, Advantages and limitations.

UNIT XI: Thermal Methods **15 h**

Thermogravimetric analysis (TGA): Principle, Instrumentation, working function of each component, applications of TGA, Study of oxalates, nitrates and chromates by TGA. Determination of carbon black in polythene.
Differential thermal analysis (DTA): Principle, Instrumentation, Methodology, applications. Differential thermogram of sulphur. TG and DTA of manganese phosphine monohydrate.
Differential scanning calorimetry (DSC): Principle, instrumentation, power compensated DSC instruments and Heat flow DSC instruments, Methodology, DSC experiment calibration and data analysis. Applications determination Glass transition temperatures and heat capacities, problems based onThermal Techniques:
Thermometric titrations: Principle, apparatus, applications to acid base, precipitation, complexometric, redox and non-aqueous titrations.
Combined thermal instruments: Introduction to TGA/MS and TGA/FTIR, High resolution TGA, Microthermal analysis.

UNIT XII: Advanced Mass spectrometry **15 h**

Mass Analyzers: Quadruple, Ion traps, Time of flight (TOF) mass analyzers
Mass Spectrometry / Mass Spectrometry: Tandem Mass Spectrometry, Instrumentation, Applications.
Hyphenated Techniques: **GC-MS** Principle, instrumentation, Interfaces- Direct coupling interface and open split interface. Application based on gas chromatography/mass spectrometry-Analysis of metabolite of drug Imipramine. **LC-MS-** principle, Instrumentation – Interfaces-Moving belt interface, particle beam interface, thermospray interface, Electrospray interface, atmospheric pressure chemical ionizationinterface. **ICP – MS** - Principle Instrumentation, and Applications.
Matrix-assisted laser desorption/ionization-Time of flight Mass spectrometry (MALDI-TOF-MS): Principle, Matrix, Sample Preparation for MALDI-MS - Dried droplet Crystallization, Thin layer method, Sandwich Crystallization, Instrumentation, Applications.

SUGGESTED BOOKS

1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York.
2. Instrumental Methods of Chemical Analysis, H. Kaur.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson EducationLtd.
4. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
5. Instrumental Techniques for Analytical Chemistry, Frank Settle.
6. Principles of Analytical Chemistry, M. Valcarcel.
7. Solid State Chemistry and its Applications, *West.*
8. Introduction to Solids, Azaroff.
9. Solid State Chemistry, D.K. Chakrabarthy
10. Physical Methods in Advanced Inorganic Chemistry, Hill and Day.
11. Instrumental Methods of Analysis, Sixth edition, CBS Publishers, Willard, Merrit, Dean,and Settle.
12. Mass spectrometry for Chemists and Biochemists, Robert A.W Johnstone and Molcolm. E.Rose,second Edn.
13. Physical methods for Chemists, Russell S. Drago second edition, Saunders Collegepublishing 1992.

14. Structural methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H Rankin and S.Craddeck, ELBS.
15. Mass Spectrometry Basics, Herbert, Christopher G.; Johnstone, Robert A.W., CRC Press.
16. Mass Spectrometry-A Textbook by Jürgen H. Gross, © Springer-Verlag Berlin Heidelberg 2004,Printed in Germany.
17. Matrix-assisted laser desorption/ionization - https://en.wikipedia.org/wiki/Matrixassisted_ laser_desorption/ionization

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER-VII
Practical

PAPER VI (ICY-751) INORGANIC CHEMISTRY-III

Teaching hours-4/week **Credits 2**

Synthesis and Characterization of Metal Complexes and Separation methods

1. Separation Methods
   i. Separation of Fe^{3+} and Ni^{2+} using tri-n-butyl phophite (TBP) from HCl medium (Solvent extraction)
   ii. Determination of cations by paper chromatography; Co(II), Ni(II) and Cu(II)
   iii. Separation of Fe(III) and Al(III) by column chromatography
   iv. Determination of capacity of an ion exchange resin.
   v. Separation of Fe^{3+} and Ni^{2+} using strongly basic anion resin.
   vi. Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+} ions.

Suggested Books :

1. Practical Inorganic Chemistry, G. Marr and B. W. Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe, 2nd edn John Wiley & Sons.
3. Experimental Inorganic/Physical Chemistry, M. A. Malati, Horwood Publishing, Chichester, UK (1999)
4. Analytical Chemistry Theory and Practice by R.M. Verma 3rd Edn.CBS Publishers &Distrbutors1994.
5. Comprehensive Experimental Chemistry by V.K. Ahluwalia et.al New Age Publications 1997.

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PAPER VII (ICY-752) ORGANIC CHEMISTRY-III

Teaching hours-4/week **Credits 2**

Synthesis of organic drug molecules & TLC

Organic Synthesis:

2-Phenyl indole (Fischer indole synthesis), 2,5-Dihydroxy acetophenone (Fries reaction), Benzilic acid from benzil (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction),

Drug Synthesis:

Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone,FIuorescien, 4-Aminobenzene sulfonamide, antipyrineand phenothiazine

Purity of the all the synthesied compounds monitered by TLC

(A) Laboratory synthesis of the following compounds: 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

(B) Isolation of the following natural products: Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

(C)Thin layer chromatography: Thin layer chromatography: Determination of purity (All the above preparations), monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the Rf values of known standards.

Reference books:

1. Practical organic chemistry by Mann & Saunders.
2. Text book of practical organic chemistry by Vogel.

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PAPER VIII (ICY-753) PHYSICAL CHEMISTRY-III

Teaching hours-4/week **Credits 2**

(A) Chemical Kinetics

I) $K_2S_2O_8$-KI reaction by colorimetry

(i) Overall order of the reaction
(ii) Order with respect to $K_2S_2O_8$ using initial rate method
(iii) Order with respect to KI using initial rate method
(iv) Order with respect to KI using isolation method

II) $K_2S_2O_8$-KI clock reaction

(i) Overall order of the reaction
(ii) Order with respect to $K_2S_2O_8$ using initial rate method
(iii) Order with respect to KI using initial rate method
(iv) Order with respect to KI using isolation method

(B)Instrumentation - Potentiometry

I) Acid –Base titrations

(i) Strong acid vs Strong base
(ii) Weak acid vs Strong base
(iii) Mixture of strong and weak acids vs strong base
(iv) Dibasic acid vs strong base
(v) Tribasic acid vs strong base

(II) Redox titrations

(i) Fe(II) vs $K_2Cr_2O_7$
(ii) Fe(II) vs $KMnO_4$
(iii) Fe(II) vs Ce(IV)
(iv) KI vs KMnO4
(v) Fe(II)+V(V) vsCe(IV)

(III) Precipitation titrations

(i) KCl vs $AgNO_3$
(ii) KI vs $AgNO_3$
(iii) KSCN vs $AgNO_3$
(iv) KCl + KI vs $AgNO_3$
(v) KI+KSCN vs $AgNO_3$

(IV) Complexometric titrations

(i) Fe(III) vs EDTA

References:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, AdarshGulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

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PAPER IX (ICY-754) PHYSICAL CHEMISTRY-3

Teaching hours-4/week **Credits 2**

Laboratory preparation and characterization of 3d transition metal complexes

i. $VO(acac)_2$
ii. $CoCl_2(Py)_2$
iii. $Na[Cr(NH_3)_2(SCN)_4]$
iv. $K_3[Cr(C_2O_4)_3]\ 3H_2O$: UV, IR, TGA and estimation of oxalate.
v. *Trans*-bis(glycinato)copper(II): IR, estimation of Cu by iodometry
vi. $Fe(acac)_3$: FTIR
vii. MnO_2 nano particles; SEM, TEM

PALAMURU UNIVERSITY
M.Sc. Integrated Chemistry
SEMESTER VIII

PAPER I (ICY-801) Skill Enhancement Course (SEC VI)

Teaching hours-2/week **Credits 2**

Intellectual Property Rights

Unit I: Introduction to IPR
Unit II: Patent Search and IP Reports Generation

Unit I: Introduction to IPR **15 h**

Introduction : Legal Rights and obligations, Concept of Property, Kinds of Property, General concept and Significance of Intellectual Property (IP), Intellectual Property Rights (IPR), Intellectual property, Introduction to IPR, contents of IPR and their protection, Recent Developments, IP Organizations.

Introduction to Patents, Trademarks, Copyrights, Trade secrets, Industrial designs and Geographical indications.

International organizations & treaties: introduction to various conventions and organizations, Paris Convention, World Trade organization (WTO)

Unit II: Patent Search and IP Reports Generation **15 h**

What is a patent search. Who needs a patent search. Patent Search Types and Methodologies, Novelty Searches, Validity Searches, Infringement Searches, State-of-the-art searches.
Searching in Patent Databases:
Free search databases: USPTO, EPSPACE, WIPO, FreePatentsOnline, FreshPatents and JSPTO, Paid search databases: Micropat, Delphion, DialogPro, Patent Optimiser, Aureka and PatentCafe, Patent Filing and Drafting, Patent filing procedures, Indian patent act, patent drafting, PCT applications, provisional and complete specifications.

References

1. Fundamentals of Jurisprudence by Dhyani, Allahabad Publication, Central Law.
2. Jurisprudence of Legal Theory by Dwivedi S.P. Allahabad Central Law Agency.
3. Text Book on Jurisprudence by Hilari WC Cobrey, Oxford Publications.
4. Treaties on Intellectual Property Rights by Blackstone
5. W.T.O. by Myneni, Asia Law House.
6. W.T.O. by Vasudeva, Minerva Publications, Delhi.
7. Law of Practice of Intellectual Property in India by VikasVashistha, Bharat Law Publications, Delhi.
8. Intellectual property rights by B L Wadhera, Universal Law Publications.
9. Trade Marks Act by Mittal, Eastern Book Company.
10. Patent Law by Narayana P, Eastern Book Company.
11. Intellectual Property Rights by Cornish, Universal Publications.

PALAMURU UNIVERSITY
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SEMESTER-VIII

Paper-II (ICY-802) INORGANIC CHEMISTRY-IV

Teaching hours-4/week **Credits 4**

Bioinorganic Chemistry

UNIT-XIII: Metal ions Interactions with Nucleic acids and their constituents
UNIT-XIV: Transport of Electrons and Metal ions
UNIT-XV: Metallo-Enzymes of Iron, Zinc and Nickel
UNIT-XVI: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese

UNIT-XIII: Metal ions Interactions with Nucleic acids and their constituents **15 h**

Nucleic Bases, Nucleosides and Nucleotides. Proton Binding Sites of Nucleic Acid Constituents-Purineand Pyrimidine Bases, Nucleosides and Nucleotides. The covalent structure of polynucleotides, secondary structure of DNA: The double helix anti and syn conformations of nucleotides. B, A, & Z forms of DNA. General Factors that influence Metal Ion Binding Sites in Solution – Specific Metal Ion Binding to Nucleic Bases, Nucleotides and Nucleosides in Solution: Stability of Phosphate- Metal ion complexes, Metal binding Metal Ion Complexes, Metal Binding Sites in Nucleosides, Nucleotide - Metal Ion Interactions – Intra-molecular Equilibrium Constant KI, Percentage of Closed Isomers - Outer Sphere and Inner Sphere Isomers of M-ATP Complexes and Metal Ion Nucleic Base Interactions. *Metal-DNA and RNA Interactions*: Potential Binding Sites (Elementary Treatment) – Influence of Metal Ions on Stability of Nucleic Acids.

UNIT-XIV: Transport of Electrons and Metal ions **15 h**

Transport of Electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe,3Fe, 4Fe, 8Fe Proteins)-High Potential Iron-Sulphur Proteins – Structural and Spectral features of Iron-Sulphur Proteins -Electron-transport by Cytochromes, Azurin and Plastocyanin - Importance of Structures of Azurin and Plastocyanin in facilitating Rapid Electron Transport, acotinase- Fe-S enzyme.

Transport and Storage of Metal Ions: Iron-Transport by Transferrin and Siderophores – Ferritin in IronStorage - Transport of Na^+ and K^+ across Cell Membranes by Na^+- K^+ ATPase - Transport of Calciumacross Sarcoplasmic Reticulam by Ca^{2+}-ATPase.

UNIT-XV: Metallo-Enzymes of Iron, Zinc and Nickel **15 h**

Iron Enzymes: Structural and Mechanistic Aspects of Cytochrome P450, Cytochrome oxidase,Catalaseand Peroxidase - Role of the Metal Ion.

Zinc Enzymes: Structural and Mechanistic Aspects of Carbonic Anhydrase, CarboxyPeptidase,Leucin –aminopeptidase, Thermolysin, Alcohol Dehydrogenase - Role of Zinc.

Nickel Enzymes: Urease, Hydrogenase and Factor F430: Reactions Catalyzed, MechanisticAspects.

UNIT-XVI: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese **15 h**

Cobalt Enzymes: Cobalt in Vitamin B12 - Structural Features of Vitamin B12 with reference tocoordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B12 and ActiveEnzyme forms - Types of Reactions Catalysed by i) Methyl Cobalamin ii)DeoxyadenosylCobalamin -Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA - Role of the Apoenzyme – Uniquefeatures of Cobalt to suit Vitamin B12.

Copper Enzymes: Types of Copper in Biological Systems - Structural and Mechanistic Aspects ofSuperoxide Dismutase, Laccase and Galactose oxidase.

Molybdenum Enzymes: Biological Roles and Mechanistic Aspects of Nitrogenase, Xanthineoxidase andSulfite oxidase.

Manganese Enzymes: Arginase, Water – oxidase.

SUGGESTED BOOKS

1. Biochemistry - Geoffrey L. Zubay.
2. Biochemistry - Mary K. Campbell. (added these books)
3. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University ScienceBooks, CaliforniaUSA 1994.
4. Principles of Bioinorganic Chemistry, S.J. Lippard and M.Berg University ScienceBooks, California1994.
5. Biological Chemistry of Elements, J.J.R. Franstodasilva and R.J.P. Williams OxfordUniversity Press1991.
6. Metal Ions in Biological Systems (Series), Ed. H. Sigel Marcel Dekkar, New York
7. Inorganic Biochemistry, J.A. Cowan, VCH publishers 1993.
8. Advances in Inorganic Biochemistry, edited by G.L.Eichorn&Marzilli
9. Bioinorganic Chemistry, Vol-I edited by G.L.Eichorn.
10. Interactions of metal ions with nucleotides and nucleic acids and their constituents Helmut SigelChem. Soc. Rev., 1993,22, 255-267.

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Paper-III (ICY-803) ORGANIC CHEMISTRY-IV

Teaching hours-4/week **Credits 4**

Modern Organic Synthesis

Unit XIII: Asymmetric synthesis
Unit XIV: Synthetic strategies
Unit XV: New Synthetic reactions
Unit XVI: New techniques and concepts in organic synthesis

Unit XIII: Asymmetric synthesis **15 h**

Introduction: Brief revision of classification of stereo selective reactions

Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chiraility and Pro-R, Pro-S, Re and Si. Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.

Analytical methods: % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule.
Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2.
Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphincatalyst.
Asymmetric aldolreaction: Diastereoselectivealdol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxelmodel.

Unit XIV: SyntheticStrategies **15 h**

Introduction:Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involvingchemoselectivity, regioselectivity, reversal of polarity and cyclizations. .
Order of events: S-Salbutamol, Propoxycaine.
One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols,ethers and sulphides.
Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.
Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.
Control in carbonyl condensations: oxanamide and mevalonic acid.
Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, longifoline.

Unit XV: New Synthetic reactions **15 h**

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira crosscoupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions,Julia-Lythgoe olefination and Peterson's stereoselective olefination.
3. Multicomponent Reactions:Ugi,Passerini, Biginelli, Bergman and Mannichreactions.
4. Ring Formation Reactions:Pausan-Khand reaction, Nazerov cyclisation.
5. Click Chemistry:Click reaction, 1,3-dipolar cycloadditions.
6.Metathesis:Grubb's 1st and 2nd generation catalyst, Olefin cross coupling Metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.
7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction,Stork-enamine reaction and Michael reactions.

Unit XVI: New techniques and concepts in organic synthesis **15 h**

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellmanresin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2. Solid phase oligodeoxynucleotidesynthesis: Phosphotriester, phosphatetriester and phosphoramidite pathway

3. Oligosaccharide synthesis: Glycosidation: cylicoxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.

4. Phase Transfer catalysis: Onium and crwon ethers as PTC.

5. Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization cyclisation, elctrocylic-Diels Alder reaction.

6. Baldwin Rules:Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

7.Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine.

8) Determination of absolute configuration: Mosher's method.

Reference Books:

1. Asymmetric synthesis by Nogradi

2. Asymmetric organic reactions by J D Morrison and H S Moscher

3. Principles in Asymmetric synthesis by Robert E. Gawley&Jeffreyaube

4. Stereo differentiating reactions by Izumi

5. Some modern methods of organic synthesis by W Carruthers

6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R AAtken

7. Organic synthesis by Michael B Smith

8. Organic Synthesis-The disconnection approach by S Warren

9. Organic Synthesis by C Willis and M Willis

10. Problems on organic synthesis by Stuart Warren

11.Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren

12.The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng

13. Name reactions by JieJacj Li

PALAMURU UNIVERSITY
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SEMESTER-VIII

Paper-IV (ICY-804) PHYSICAL CHEMISTRY-IV

Teaching hours-4/week **Credits 4**

Unit XIII: Angular momentum and approximate methods
Unit XIV: Polymerization and Kinetics of polymerization
Unit XV: Non-equilibrium Thermodynamics
Unit XIII: Bonding in molecules

Unit XIII: Angular momentum and approximate methods 15 h

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L 2 and L z and the eigen values. Magnitude and orientation of angular momentum vectors. Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Approximate methods- The variation method. Construction of variation function by the method of linear combinations. H and He atom. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom. Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions. Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals (STOs).

Unit XIV: Polymerization and Kinetics of polymerization 15 h

Classification of polymers. Types of polymerization. Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of cationic, anionic polymerization, coordination polymerization, linear stepwise polymerization. copolymerization reactions and copolymer composition. Reactivity ratios and their determination.

Alfrey and Price Q-e scheme for monomer and radical reactivity. Block and graft copolymers. Polymerization in homogeneous and heterogeneous systems. Techniques of polymerization- Bulk, solution, suspension and emulsion polymerizations.

Unit XV: Non-equilibrium Thermodynamics 15 h

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow. Fluxes and forces. Linear flux-force relations. Phenomenonological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations. Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle

of minimum entropy production. Irreversible thermodynamics as applied to biological systems - examples. Application to thermoelectric circuits. Seebeck and Peltier effect.

Unit XVI: Bonding in molecules **15 h**

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of H_2 molecule. Calculation of energy. MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations. MOs of H_2O. Concept of hybridization – sp, sp^2 , and sp^3 hybrid orbitals. Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry.

Introduction to extended Huckle Theory, extension of the Huckle's approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

SUGGESTED BOOKS

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
6. Text book of Biochemistry by Stryer, W.H. Freeman & Co Ltd
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
9. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
10. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
11. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
12. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and professional
13. Materials science and engineering an introduction by William D Callister, Jr. Wiley Publ
14. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley
15. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS
16. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons
17. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London 2000).
18. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
19. Coulson's Valence, R. McWeeny, ELBS

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SEMESTER-VIII

PAPER V (ICY-805) ANALYTICAL TECHNIQUES AND SPECTROSCOPY-IV

Teaching hours-4/week **Credits 4**

UNIT-XIII : AAS, AES, ICP-AES
UNIT-XIV : Multinuclear NMR
UNIT-XV : Mossbauer and Nuclear Quadrupole Resonance Spectroscopy
UNIT-XVI : Green Chemistry

UNIT-XIII: AAS, AES, ICP-AES 15 h

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences – chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis.

Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, interferences, evaluation methods, Application in quantitative analysis.

Flame Photometry: Principle, Theory, Instrumentation and Applications

Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Application of ICP-AES, Comparison with AAS.

UNIT-XIV: Multinuclear NMR and ESR of Transition metal complexes 15 h

Virtual Coupling and its importance in study of Metal Complexes $[Pd\{P(CH_3)_3\}_2I_2]$. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$. NMR Time Scale and its use in studying Stereo chemical Non–rigidity (PF_5, $[Rh(PR_3)_5]^+$, $[Fe\{Cp\}_2(CO)_2]$) - ΔR, the Ring Contribution to ^{31}P Chemical Shifts –Metal and Chelate size on ΔR.

Applications of ^1H, ^{13}C, ^{19}F, ^{31}P and ^{15}N to simple inorganic and Coordination Compounds (1) **^{1}H-NMR**: $PtHCl(PEt_3)_2$, $Pt(NH_3)_3(CH_3)_3$, BH_4^-, NH_4^+, CH_3CN, $[6h\text{-}C_7H_8Mo(CO)_3]$, $[7h\text{-}C_7H_7Mo(CO)_3]^+$, B_2H_6; $^{29}SiH_3SiH_3$, (2) **^{19}F**: BF_4^-, H_2PF_3 (3) **^{31}P**: $Mo(CO)_3(PPh_3)_3$, $[Rh(PPh_3)_3Cl]$, trans-$[PtCl_4(PEt_3)_2]$, $^{31}PF_2H(^{15}NH_2)_2$ (4) **^{13}C**; $[4h C_8H_8Ru(CO)_3]$, $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, $FeICp(CO)_{12}$, $[^{13}C^{15}NCo(DH)_2Pyridine]$. $^{13}C\{^1H\}$ NMR spectrum of σ-bonded C_6H_5 ligand.

Applications of ESR to Metal Complexes: ESR Spectra of d^1–d^9 Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Intensities of 'g ∥ and g ⊥ peaks. Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicylaldimine. $[(NH_3)_5CoO_2Co(NH_3)_5]^{5+}$, Cu(II)-diethyldithiophosphinate, Vanadyldithiophsphinate, Copper(II) tetraphenylporphyrin, Co(II)-phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from ESR spectral data in - i) MnF_6^{4-}, ii) CoF_6^{4-} and CrF_6^{3-}. ESR spectra of dinuclear Cu(II) complexes.

UNIT-XV : Mossbauer and Nuclear Quadrupole Resonance Spectroscopy **15 h**

Mossbauer Spectroscopy: Principle, Experimental Considerations and Presentation of the Spectrum -Isomer Shifts – Quadrupole splitting and Magnetic hyperfine splitting - Selection Rules.

Applications:

Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes - π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds -Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins.

Tin Compounds: Tin Halides and Organotin Compounds.

Iodine Compounds: Isomer Shifts of ^{127}I and ^{129}I - Applications to Alkali metal iodides and Molecular Iodine. Mossbauer spectra of IF_6^- and IF_6^+

Nuclear Quadrupole Resonance Spectroscopy: Principle, nuclear quadrupole resonance experiment, Structural information from NQR spectra- $PFCl_4$, PCl_4Ph, $Ga_2Cl_7^-$ and $TeCl_4$ Interpretation of nuclear quadrupole coupling constants.

UNIT-XVI: Green Chemistry **15 h**

Principles and concepts of green chemistryIntroduction, sustainable development and green chemistry, atom economy, atom economic reactions,rearrangement reactions, addition reactions, atom uneconomic reactions- substitution reactions,elimination reactions, Wittig reactions.Reducing toxicity, measuring toxicity.Organic solvents: Environmentally benign solutions: Organic solvents and volatile organic compounds,solvent free systems, super critical fluids- supercritical carbon dioxide and supercritical water. Water as areagent solvent, water based coatings.Industrial case studies: A brighter shade of green – greening of acetic acid, Vitamin C synthesis –enzymeroutes. Polythene manufacture-metallocene catalysis.

SUGGESTED BOOKS

1. Instrumental Techniques for Analytical Chemistry, Frank Settle.
2. Principles of Analytical Chemistry, M. Valcarcel.
3. NMR in chemistry - A multinuclear introduction by William Kemp
4. Spectroscopic identification of organic compounds by P S Kalsi
5. Introduction to organic spectroscopy by Pavia
6. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
7. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
8. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
9. NMR spectroscopy by H.Gunther
10. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS.
11. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.

12. Physical Methods for Chemists, Russell S. Drago Second edition, SaundersCollege Publishing, 1992.

13. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.

14. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London,1971.

15. Principles of Instrumental Analysis, Skoog, Holler and Nieman.

16. Physical Methods in Advanced Inorganic Chemistry, Hill and Day

17. Magneto Chemistry, Dutta &Shyamal Oxford Chemistry Primers, Vol 62 A.S. Matlack:

18. Introduction to Green Chemistry, Marcel Deckkar, (2001).

19. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).

20. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

21. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers

22. P.T. Anastes& J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).

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M.Sc. Integrated Chemistry
SEMESTER-VIII
Practical
PAPER VI (ICY-851) INORGANIC CHEMISTRY- IV

Teaching hours-4/week Credits 2

I Colorimetry
1. Determination of blood cholesterol
2. Determination of Glucose
2. Determination of Paracetamol

II Fluorimetry
1. Determination of Riboflavin

III Flame photometry
1. Determination of Na
2. Determination of K

Suggested books:

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememanet. JohnWiley & Sons 1984.
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rd Edition, Elbs Publication 1969.
3. Vogel's Text Book of Quantitative Inorganic Analysis Jeffery etal 4th edition, ElbsPublications 1988.
4. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
5. Analytical Chemistry Theory and Practice by R.M. Verma 3rd Edn.CBS Publishers &Distrbutors1994.
5. Comprehensive Experimental Chemistry by V.K. Ahluwalia et.al New Age Publications 1997.
7. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2 nd edn. 1996.
8. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rd EdnElbs Publication 1969.
9. Quantitative Analysis by Day and Underwood Prentice Hall (India) VI Edn.
10. Analytical Chemistry Theory and Practice by R. M. Verma 3rd Edn.CBS Publishers &Distrbutors1994.
11. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001
12. Medical Laboratory Technology – Mukherjee,McGraw Hills, 1988.

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Practical

PAPER VII (ICY-852) ORGANIC CHEMISTRY- IV

Teaching hours-4/week Credits 2

Paper CH (O) 352P: Separation and identification of organic compounds & Column Chromatography

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil. hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of **09** mixtures should be separated and analyzed by these procedures.

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Practical

PAPER VIII (ICY-853) PHYSICAL CHEMISTRY-IV

Teaching hours-4/week **Credits 2**

Kinetics and Instrumentation

(A) Acetone – Iodine reaction by volumetry
(i) Order with respect to iodine
(ii) Order with respect to acetone
(iii) Order with respect to H^+
(B) Acetone – Iodine reaction by spectrophotometry
(i) Order with respect to iodine
(ii) Order with respect to acetone
(iii) Order with respect to H^+
(C) Saponification of ethyl acetate by volumetry
(D) Saponification of ethyl acetate by conductometry
(i) Overall order of the reaction
(ii) Order with respect to ethyl acetate
(iii) Order with respect to NaOH

pH-metry

(1) Strong acid vs Strong base
(2) Weak acid vs Strong base
(3) Mixture of strong and weak acids vs strong base
(4) Dibasic acid vs strong base
(5) Tribasic acid vs strong base
(6) Determination of dissociation constants of monobasic/dibasic acids by Albert- Serjeant method
(7) Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane

(8) Determination of pKa and pKb of glycine
(9) Determination of stability constant of metal complex

References:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, AdarshGulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

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PAPER IX (ICY-854) GENERAL CHEMISTRY-4

Teaching hours-4/week Credits 2

Spectroscopic methods of Analysis

Spectrophotometry

1. Determination of Manganese in steel
2. Determination of chromium
3. Determination of Manganese and chromium simultaneously.
4. Determination of composition of Complex by Job's Method and Mole ratio Method in the following:
   (i) Cu (II)-EDTA
   (ii) Fe (II) – o-Phen
5. Determination of Fluoride by Zirconium Alizarin Method

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SEMESTER IX

PAPER I (ICY-901) Skill Enhancement Course (SEC-VII)

Teaching hours-2/week **Credits 2**

Research Methodology

Unit I: Introduction to Research Methodology
Unit II: Chemical Information Sources and Searches

Unit I: Introduction to Research Methodology: **15 h**

Definition, objectives of research, types of research- significance of research, research and scientific method, importance of knowing how research is done.

Research process - formulating the research problem, extensive literature survey, development of working hypotheses, preparing the research design, determining sample design, collecting the data, execution of the project, analysis of data, hypothesis-testing, generalizations and interpretation, preparation of the report or the thesis.
Criteria of good research, problems encountered by researchers in India.
Defining the research problem, selecting the problem, necessity of defining the problem.
Research design, need for research design, features of a good design, Basic principles of experimental designs

Unit II: Chemical Information Sources and Searches **15 h**

Advantage/Limitation of computer searching strategies and tactics for searches
Types of Publications: Journals, technical reports, Patents, Conference Papers, Dissertations, Electronic Publications –
Types of databases – Public databases; NCBI, RCSB, CSD, SWISS-PROT and Paid databases CAT'STN and SciFinder - Computer searching of chemical abstracts – Web-based cross platform solutions for Cheminformatics and chemical communications (BLAST, ClustalW, RasMol, SAVES) – JChemBase – Keyword-based general bibliographic searches – Chemical connectivity and structure searches (2D) – Chemical structure, property and shape based searches (3D) – Searching for the synthesis (or) reactions of specific compounds or classes of compounds

Reference Books

1. Research Methodology- Methods and techniques, C. R. Kothari, New Age International (P) Ltd., Publishers.
2. Chemical Information Sources by Institute of Cheminformatics Studies.
3. Geer LY, Marchler-Bauer A, Geer RC, Han L, He J, He S, Liu C, Shi W, Bryant SH. The NCBI BioSystems database. Nucleic Acids Res. 2010
4. An Introduction to Computer Searching of Chemical Abstracts STN International Version
5. https://www.cas.org/products/scifinder.

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SEMESTER-IX

PAPER II (ICY-902) INORGANIC CHEMISTRY-V

Teaching hours-4/week **Credits 4**

Organo Metallic Chemistry of Transition Metal Complexes

UNIT-XVII: Mono,Di and Trihapto Complexes
UNIT-XVIII: Tetra, Penta, Hexa, Hepta and Octahapto Complexes
UNIT-XIX: Catalytic Role of OTMC-I
UNIT-XX: Catalytic Role of OTMC-II

UNIT-XVII: Mono, Di and Tri hapto Complexes **15 h**

Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number ofelectrons donated by the Ligand. 16 and 18 electron rules. Electron countingcovalentand ionic models. η1– Complexes : General methods of Preparation –Bonding of Ligand to Metal :αand βInteraction andagostic interaction– Stability and decomposition pathways –η1 Complexes –Tertiary Phosphine –Transition Metal Alkyl and Aryl Complexes of Pt – Ortho-effect – Bonding in Metal – Carbene andCarbyne Complexes. η2 –Complexes: General methods of preparation of Metal – Alkene Complexes –Structure and Bonding in η2 Complexes-Zeises salt – Trans Effect – Rotation of Olefin around Metal-Olefin Bond. η3 - Complexes: Metal-Allyl Complexes – General Preparative Routes – Structure andBonding in η3 Allyl Complexes – Fluxionality.

UNIT-XVIII: Tetra, Penta,Hexa,Hepta and Octahapto Complexes **15 h**

η4 Complexes: Structure and Bonding in η4 Complexes –Butadiene and Cyclobutadiene Complexes. η^5– Complexes: General methods of Preparation – Bis (η5-cyclopentadienyl) metal complexes(Metallocenes) – Ferrocene: Structure and Bonding –Reactions of Ferrocene – Mechanism of Electroplilic substitution – Friedel Crafts acylation, alkylation, nitration, halogenation and Metallation Reactions.η^6Complexes : Metal –Arene Complexes – Dibenzenechromium – Preparation, Structure and Bonding inBis(arene)-Metal Complexes – Reactions. η^7Complexes : Preparation , Structure and Reactions of η^7–C_7H_7 Complexes. η^8Complexes : C_8H_8 as a Ligand – Cyclooctatetraene Complexes – Preparation,Structure and Bonding in Uranocene.

UNIT-XIX: Catalytic Role of OTMC-I **15 h**

Oxidative addition and Reductive Elimination: Stereochemistry and Mechanism of Oxidative Addition – Insertion Reactions – Hydrogenation of Olefins –Transfer Hydrogenation –Hydrosilation of Olefins – Isomerisation of Olefins – Ziegler –Natta Polymerization of Olefins – Oligomerization of ButadieneAlkene Metathesis. Dupont-1, 4-hexadiene synthesis.Oxidation of Olefins to Carbonyl Compounds –Oxidation of Hydrocarbons to Alcohols and Acids – Oxidation of Aldehydes, Cyclohexanol,Cyclohexanone, p-Xylene.

UNIT-XX: Catalytic Role of OTMC- II **15 h**

Reactions of Carbon monoxide and Hydrogen:Hydroformylation – Carbonylation –Syngas- Water gasshift Reaction (WGS) – Reactions of Syngas.Applications of Metal Clusters inCatalysis:Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]$ – , Hydrogenation of Olefins. Use of$[Fe_4C(CO)14]$ as a model for Fischer – Tropsch process. Recent Developments in Homogenous Catalysis:Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalyzed Reactions under PhaseTransfer Conditions: Hydrogenation. Bio Catalysis : Enzyme Analogue Catalysis: Introduction, Examplesof Enzymatic Conversions, Reduction of >C=O and >C=C< bonds, Templates: Introduction, MetalCations as Templates, Covalent molecules as Templates, External and Internal Templates – Homogeneous Catalysts and theirHeterogenization or Immobilization by Aqueous Catalysis.

SUGGESTED BOOKS :

1.Organometallics-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH
2.Organotransition Metal Chemistry Fundamental Concepts and Applications, John AkioYamamato,Wiley & Sons.
3.Homogeneous Catalysis by Metal Complexes, M MTaqui Khan and A E Martel
4. Applied Homogenous Catalysis with Organo Metallic Compounds Vol I & II, Boy Cornillsand W A
5. Herrmann – VCH
6. Organometallic Compounds, G E Coates, M C H Green, K Wade vol II
7. Advanced Inorganic Chemistry, Cotton and Wilkinson, V & VI Ed
8. ymmetry and spectroscopy, K.Veera Reddy
9. Homogenous catalysis, G W Parshall, John Wiley & Sons, New York
10. Basic organometallic Chemistry, B.D. Gupta / A. J. Elias

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SEMESTER-IX

PAPER III (ICY-903) ORGANIC CHEMISTRY-V

Teaching hours-4/week **Credits 4**

Bioorganic Chemistry

Unit- XVII: Proteins, Nucleic acids and Lipids, introduction to metabolism
Unit- XVIII: Enzymes, Coenzymes and Vitamins
Unit- XIX: Heterocyclic Chemistry-I
Unit- XX: Heterocyclic Chemistry-II

UNIT-XVII: Proteins, Nucleic acids and Lipids, introduction to metabolism **15 h**

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins – Biological importance and classification - Primary, secondary and tertiary structure of proteins.

Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids. Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes.

Introduction to metabolism: Overview of metabolism, catabolic & anabolic processes, glycolysis citric acid cycle & oxidative phosphorylation.

UNIT-XVIII: Enzymes, Coenzymes and Vitamins **15 h**

Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity –chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme

catalysis. Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

Coenzymes: Introduction. Co-factors -cosubstrates -prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes.Structure and biologicalfunctionsof coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH) ii) Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP)and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Vitamins: Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, B_1, and B_2. Synthesis of vitamins - B_6, C, E and K. Structure of vitamin B_{12}.

UNIT-XIX Heterocyclic Chemistry – I **15 h**

Nonaromatic & Aromatic heterocyclics & Aromaticity

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems.Azirines, Oxiranes, Thiiranes, Diazirenes, Oxaziridines, Oxetanes. Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole,

Aromaticity: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

UNIT-XX: Heterocyclic Chemistry – II **15 h**

Five and six membered heterocyclics with two and morethan two hetero **atoms**

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyridazine, Pyrimidine, Oxazine, benzimidazole, benzoxazole and benzthiazole. Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines.Syntheis of Caffeine, theobromine and theophylline.

Larger ring and other Heterocycles :

Synthesis, structure, stability and reactivity ofAzepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, PhospholesandBoroles.

Reference Books:

1. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait

2. Lehninger Principles of Biochemistry by D L Nelson and M MCoxon

3. Outlines of Biochemistry by Conn and Stumpf

4. Enzyme structure and mechanism by Fersht and Freeman

5. Enzymes for green organic synthesis by V.K. Ahluwalia

6. Biotransformations in Organic Chemistry by K Faber.

7. Principles of biochemistry by Horton &others.

8. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugasand Christopher Penney.

9. Concepts in Biotechnology by D. Balasubramanian & others

10. Chemistry and physiology of the vitamins by H.R. Rosenberg.

11. Heterocyclic Chemistry, T. Gilchrist

12. An introduction to the Chemistry of heterocyclic compounds, R.M. Acheson

13. Heterocyclic Chemistry, J.A. Joule & K. Mills

14. Principles of Modern Heterocyclie Chemistry, A. Paquette

15. Heterocyclic Chemistry, J,A. Joule & Smith

16. Handbook of Heterocyclic Chemistry, A.R. Katritzky

17. The aromaticity III level, units 17-19 British open university volumes

18. Aromatic character and aromaticity by G.M.Badger

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SEMESTER-IX

PAPER IV (ICY-904) PHYSICAL CHEMISTRY-V

Teaching hours-4/week **Credits 4**

Unit-XVII: Nanomaterials & Non Linear Optical materials
Unit-XVIII: Lasers in Chemistry
Unit-XIX: Phase-transfer catalysis (PTC)
Unit-XX: Corrosion and its control

Unit-XVII: Nanomaterials & Non Linear Optical materials **15 h**

Introduction to nanomaterials, Classification of nanomaterials: Zero Dimensional, 1D, 2,D 3D with examples. Preparation of nanomaterials: Top-down approach: Lithography, Ball Billing, Bottom Up: Physical Vopour deposition (PVD), Chemical Vopour Deposition (CVD) Sol-gel method, Characterization of nanoparticles: (a) powder X-ray diffraction (NaCl), Transmission

electron microscopy (TEM) indexing of (hkl) values, Surface analysis: BET, BJH (derivation not required) with examples. Effect of particle size on optical properties of nanomaterials. Applications of nanonanomaterilas.
Techniques of single crystal growth – growth from solutions – growth from melts – growth fromvapour. Non-linear optical (NLO) behavior– basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.

Unit-XVIII: Lasers in Chemistry: **15 h**
General principles of laser action. Stimulated emission. Rates of absorption and emission. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonantmodes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Qswitching.Pulse modification, mode-locking.
Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.Applications of lasers in chemistry: Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – thereaction between hydrogen atoms and vibrationally excited HDO molecules.
Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra ofdiphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Unit-XIX: Phase-transfer catalysis (PTC): **15 h**
Principles of phase-transfer catalysis. PTC classification.Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions. Inverse phase transfer catalysis. Mechanism of nucleophilicdisplacement reactions.
Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC's viz., quarternary ammonium salts and crown ethers
Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature ofthe metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors,coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductorparticles, removal of organic and inorganic pollutants, for oxidation and reduction of organic
compounds.

Unit-XX: Corrosion and its control: **15 h**
Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, factors affecting corrosion- nature of metal, purity of metal, electrochemical series, over voltage, nature of oxide film, nature of corrosion product, nature of environment, effect of temperature, effect of pH, effect of oxidant, humidity. Corrosion control methods design and material selection, cathodic protection, sacrificial anode, impressed current cathode. Surface coating methods: Surface preparation, metallic coatings.
Application of metal coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Organic surface coatings-paints, constituents of paints and their functions, methods of application of paints, failure of paint films, varnishes, enamels, lacquers.

References:

1. Introduction to Nanoscience and Nanotechnology, K.K. Chattopadhyay, A. N. Banerjee, PHI Learning Private Limited.
2. Nanomaterials and Nanocomposites, Rajendra Kumar Goyal, CRC Press.
3. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons
4. Solid state chemistry and applications. A.R.West, John Wiley & Sons
5. Principles of the Solid State, H. V. Keer, New Age International
6. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
7. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
10. Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company, (2008)
11. Chemistry of Engineering Materials by C.V. Agarwal, C.P. Murthy & A. Naidu: BS publications
12. Chemistry of Engineering Materials by R.P. Mani & K.N. Mishra, CENGAGE learning
Applied Chemistry – A text book of engineering and Technology – Springar (2005)

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SEMESTER-IX

Paper-V (ICY-905) ANALYTICAL TECHNIQUES AND SPECTROSCOPY-V

Teaching hours-4/week **Credits 4**

UNIT-XVII: Data Handling
UNIT-XVIII: Surface Analysis Methods/ Microscopic analysis
UNIT-XIX: Advanced Separation Techniques
UNIT-XX: Supramolecular Chemistry

UNIT-XVII: Data Handling **15 h**

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinateerrors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard
deviation, coefficient of variation and variance), significant figures – computation rules, comparison ofresults – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regressionanalysis – method of least squares, correlation coefficient, detection limits. Calculations.

UNIT-XVIII: Surface Analysis Methods (Microscopic analysis) **15 h**

Introduction, types of surface measurements.
Photon Probe Techniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation,applications

Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Transmission Electron Microscopy (TEM) - Principle, Instrumentation, applications. Energy Dispersive X-ray Spectroscopy (EDX) - Principle, Instrumentation, applications. Electron Probe X-rayanalysis (EPXMA) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) -Principle, Instrumentation, applications.
Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation,applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle,Instrumentation (static & dynamic), applications
Scanning probe microscopy Techniques: Scanning Tunneling Microscopy – Principle, Instrumentation, applications. Atomic Force Microscopy - Principle, Instrumentation, applications.

UNIT-XIX: Advanced Separation Techniques **15 h**

Separations by extractions: Solid phase extraction- Principle, methodology, applications. Solventextraction of flow injection analysis. Applications to extractions of metal ions by chelating agents (Dithiazone, 8-hydroxy quinoline and cupferron). Organic reagents in Inorganic analysis – Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organicreagents – acetylacetone, thionyl-trifluoroacetone, tri-n-octyl phosphine oxide.
Affinity and chiral chromatography – Principle, technique, Instrumentation and applications. Size Exclusion Chromatography – Principles of gel – filtration Chromatography, Instrumentation,retention behavior, resolution, selection of gel type, applications, Ion exclusion – Principle andapplications.
Supercritical fluid chromatography (SFC) – Instrumentation of SFC, stationary and mobile phasesused in SFC, Detectors, Advantages of SFC. Technique and applications of SFC

UNIT-XX: Supramolecular Chemistry **15 h**

Host – Guest chemistry: Definition and different types of host and guests with examples – types of noncovalentinteractions – binding constants of host guest complex and thermo dynamics involved in it – designing principles of host.
Cation guest binding – binding between metal cations and macro cycles – chelate and cryptate effects –relationship between cavity size of host and cation radius and stability of resultant complexes – binding of macro cycles having secondary binding sites.
Anion guest binding – different hosts for anionic guests capable of binding through electro staticinteractions, hydrogen bonds, lewis acidic hosts – enhancement of binding strength using more than noncovalentinteractions.
Neutral guest binding – binding of neutral guest using hydrogen bonding, π - π stacking, hydrophobiceffect and charge transfer interactions – simultaneous binding of cation and anion guests – cascadeapproach, individual binding sites and zwitter ions approach –present and future applications – phasetransfer agents – separation of mixtures – molecular sensors – switches and molecular machinery.

SUGGESTED BOOKS

1. Principles of Instrumental Analysis: Holler, Skoog and Ccrouch, 6th edition ,Cengage Learning 2007.
2. Instrumental methods of chemical analysis B.K. Sharma, Goel Publishing House.
3. Instrumental Methods of analysis, Willard Mersritt, Dean and Settle, 7th edition, CBS Publishers 1986.
4. Analytical Chemistry – Gary D. Christian, 6 th ed., John Wiley and sons. Inc., New York 1994.
5. Instrumental methods of Analysis - Willard, Merit, Dean, 6 th ed., CBS Publishers & distributors, 1986.
6. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA, 1997.
7. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5 th ed., Longmann, ELBS Publications, 2000.
8. Supramolecular Chemistry – concepts and perspectives by Jean-Marie Lehn
9. Principles and methods in Supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons
10. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M. Khopkar, Narosa Publishing House

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PAPER VI (ICY-951) INORGANIC CHEMISTRY-V

Teaching hours-4/week **Credits 2**

Electro-analytical techniques

I Potentiometry : Potentiometric Titrations and Calculation of End Point Potentials for the following systems:

1) Fe^{2+} and VO^{2+} Mixture vs Ce^{4+}
2) Assay of sulphanilamide
3) Silver electrode for silver assay
4) Mixture of halide anions using Silver electrode

II pH-metry

1. Determination of CO_3^{2-} and HCO_3^- in a mixture
2. Determination of the dissociation constants of
   (i) Ethylenediamine (en)(H_2L) (ii) Glycine (HL)
3. Determination of binary constants of i) Cu(II)-en and (ii) Ni(II) – Gly Systems

III Conductometry:

1. Determination of the Composition of Cu(II)-oxine and Cu(II)-EDTA Complexes

2. Interaction of Pyrophosphate with Mg^{2+}, Ca^{2+} , Mn^{2+} and Cu^{2+}

SUGGESTED BOOKS:

1. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition Elbs Publication 1969.
2. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications
1988.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
4. Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC 1988.
5. Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York – 1996.
6. Analytical Chemistry by Gary D.Christian 6th EditionJohnWiley&SonsInc New York 1994.

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PAPER VII (ICY-952) ORGANIC CHEMISTRY-V

Teaching hours-4/week **Credits 2**

(A) Spectral Problems, drug analysis & isolations

Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR, and mass spectral data(two examples with 2D-NMR). A minimum of 20 representative examples should be studied.

(B) Estimation of the following drugs:
Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid Riboflavin(colorimetry), Ca+2 ions in Calcium gluconate injection(complexometry),

Isolation of caffeine from tea leaves, piperine from pepper, lycopene from tomatoes, curcumin from turmeric.

Reference books:
1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al

5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

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PAPER VIII (ICY-953) PHYSICAL CHEMISTRY-V

Teaching hours-4/week Credits 2

Kinetics

(A) $H_2O_2 - I^-$ Clock reaction

(i) Over all order

(ii) Order with respect to Iodide

(iii) Order with respect to H_2O_2

(iv) Order with respect to acid

(B) Oxidation of alcohols using potassium dichromate by colorimetry

(i) Order with respect to acid

(ii) Order with respect to alcohol

(iii) Order with respect to potassium dichromate

(C) Kinetics of hydrolysis of t-butyl chloride by conductometry

References:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, AdarshGulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

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PAPER IX (ICY-954) GENERAL CHEMISTRY-5

Teaching hours-4/week Credits 2

Instrumentation spectrophotometry

(i) Estimation of Cu(II) using EDTA
(ii) Estimation of Fe(III) using thiocyanate
(iii) Estimation of Fe(II) using 1,10-phenanthroline
(iv) Estimation of Fe(III) in tap water using thiocyanate by standard addition method
(v) Simultaneous determination of dichromate and permanganate in a mixture
(vi) Composition of Cu(II) – EDTA complex by Job's method
(vii) Determination of composition and Gibbs energy of formation of Fe(III)–salicylic acid complex

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Project Work (ICY-1001)

Bench work hours-25/week Credits 25

I. Bench Work
II. Project Dissertation
III. Project Seminar
IV. Project Viva