DEPART MENT OF CHEMISTRY
TRIPURA UNIVERSITY
(A Central University)
Suryamaninagar-799022
West Tripura, India

Phone: +91-381 237907
Fax: +91-381 23480;
Email:hod_chemistry@tripurauniv.

No.F.1/TU/CHEM/BGPS/10

Date: 18.05..2015

NOTICE

15th BPGS Meeting will be held on 1st June , 2015 at 11.00 AM in the Department of Chemistry, Tripura University to discuss the following agenda.

18 05 15

(Prof. R.K.Nath)
Convener
BPGS, in Chemistry
Dept. of Chemistry, T.U.

Agenda for the meeting

1. Syllabus for CBCS system (M.Sc.) New Syllabi
2. RAC for Research Scholars
3. Miscellaneous.

To

1. Prof. S. Sinha, Dean Faculty of Science, Tripura University
2. Prof. B. K. De, HOD, Physics, TU,
3. Prof. M. K. Singh, Dept. of Chemistry T.U.
4. Prof. D. Sinha, Dept. of Chemistry,
5. Dr. R. N. Dutta Purkayastha, Dept. of Chemistry,T.U
6. Dr. S. Majumdar, Dept. of Chemistry, T.U
7. Dr. U. C. De, Dept. of Chemistry, T.U
8. Dr. S. Chowdhury, Dept. of Chemistry ,T.U
9. Prof. S. Bhattacharya, Dept. of Chemistry, Jadavpur University, Kolkata
10. Prof. A. Basak, Dept. of Chemistry, IIT Kharagpur, Kharagpur
11. Prof. K. Ismail, Dept. of Chemistry, North Eastern Hill University, Shillong

Copy to: 1. Dr. B.C.Sinha, Controller of Examination, Tripura University
2. P.S. to Vice-Chancellor, Tripura University, for kind information.

5/15 BPGS Meeting held on 01.06.2015 at 11.00 am.

Members Present:

1. Prof S. Sivaji
2. Prof B. K. De
3. Prof. K. Is said, we do not exist
4. Prof M. K. Sinha
5. Prof D. Sinha
6. Dr. A. K. Bhattacharya
7. Dr. S. Majumdar
8. Dr. U. C. De
9. Dr S. Choudhury.

Resolution: Proceedings of the last BPGS meeting dt. 30.03.2015 was read out and confirmed.

Resolution adopted in the meeting are as follows:

Agenda 1 M.Sc. (Chemistry) syllabi for the I Semester under CBCS system were framed and approved. Following are the approved courses:

(1) 701C – Inorganic Chemistry - 4 credit
(2) 702C – Organic Chemistry - 2 credit
(3) 703C – Physical Chemistry - 2 credit
(4) 704C – Chemistry Practical - I: 4 credit

Further, the syllabi of the following Physical Chemistry courses for the 2nd, 3rd and 4th Semesters (Core as well as Elective) were framed and approved:

(1) 803C – 2 credit
(2) 903C – 4 credit (four credit)
(3) 1003C – 2 credit
(4) 811E – 2 credit
(5) 812E – 2 credit
(6) 813E – 2 credit
(7) 911E – 2 credit
(8) 912E – 2 credit

contd/-

(9) 913E - 2 credit
(10) 1012E - 2 credit
(11) 1013E - 2 credit
(12) 1014E - 2 credit

The syllabi for the following Organic Chemistry courses for the 2nd Semester (Core and Elective) were also framed and approved:

(1) 802C - 4 credit
(2) 808E - 2 credit
(3) 809E - 2 credit
(4) 810E - 2 credit

Agenda - 2 RAC's (Research Advisory Committee) for the following students submitted by the respective Supervisors, were discussed and approved

Name of the Student	Supervisor
1. Sukhen Bhowmik —	Dr. U. C. De
2. Minarul Islam —	Dr. S. Debnath (Supervisor)
3. Tanusree Deb —	Dr S. Debnath
4. Nandita Das —	Dr. R. N. Bhattacharjee
5. Sanjay Sarkar —	Dr R. N. Bhattacharjee
6. Aditi Bhowmik —	Prof R. K. Nath
7. Payel Mitra	Prof. R. K. Nath
8. Baptu Saha	Dr S. Chowdhury

1cc 01/6/15

Convener
Board of Post-Graduate Studies
Department of Chemistry
Tripura University
Suryamaninagar-799022

DEPARTMENT OF CHEMISTRY

TRIPURA UNIVERSITY

SURYAMANINAGAR – 793022

M. Sc. CHEMISTRY SYLLABUS

CHOICE-BASED CREDIT SYSTEM
(2015)

01.06.2015
Convener
Board of Post Graduate Studies
Department of Chemistry
Tripura University
Suryamaninagar-799127

Course Curriculum – M. Sc. in Chemistry

Course Code	Name of the Courses	Credits
Semester -I		
CHEM 701C	Inorganic Chemistry-I	04
CHEM 702C	Organic Chemistry-I	02
CHEM 703C	Physical Chemistry-I	02
CHEM 704C	Chemistry Practical-I	04
Semester - II		
CHEM 801C	Inorganic Chemistry-II	02
CHEM 802C	Organic Chemistry-II	04
CHEM 803C	Physical Chemistry-II	02
CHEM 804C	Chemistry Practical-II	04
Elective		
CHEM 805E	Spectroscopic methods in inorganic Chemistry	02
CHEM 806E	Nuclear and Radiation Chemistry	02
CHEM 807E	X-ray Crystallography	02
CHEM 808E	Pericyclic and Organic Photo Chemistry	02
CHEM 809E	Chemistry of Bio Molecules	02
CHEM 810E	Medicinal Chemistry-I	02
CHEM 811E	Irreversible Thermodynamicsand Non-equilibrium Thermodynamics	02
CHEM 812E	Spectroscopy-I	02
CHEM 813E	Polymer Chemistry	02
Semester - III		
CHEM 901C	Inorganic Chemistry-III	02
CHEM 902C	Organic Chemistry-III	02
CHEM 903C	Physical Chemistry-III	04
CHEM 904C	Chemistry Project-I	04
Elective		
CHEM 905E	Metal Clusters	02
CHEM 906E	Inorganic Polymers	02
CHEM 907E	Analytical Techniques in Chemistry	02
CHEM 908E	Chemistry of Macromolecules	02
CHEM 909E	Chromatographic Techniques	02
CHEM 910E	Enzyme Chemistry	02
CHEM 911E	Surface Chemistry	02
CHEM 912E	Statistical Thermodynamics	02
CHEM 913E	Advanced Group theory	02
Semester - IV		
CHEM 1001C	Inorganic Chemistry-IV	02
CHEM 1002C	Organic Chemistry-IV	02
CHEM 1003C	Physical Chemistry-IV	02
CHEM 1004C	Supra-molecular and Nano Chemistry	02
CHEM 1005C	Chemistry Project-II	04
Elective		
CHEM 1006E	Organometallics and Catalysis	02
CHEM 1007E	Bio-Inorganic Chemistry	02
CHEM 1008E	Environmental and Green Chemistry	02
CHEM 1009E	Advanced Spectroscopic Techniques	02
CHEM 1010E	Chemistry of Natural Products	02
CHEM 1011E	Medicinal Chemistry-II	02
CHEM 1012E	Photochemistry	02
CHEM 1013E	Fortran and C, C+, C++ Programming	02
CHEM 1014E	Statistical Mechanics	02

Date 01.06.2015

Convener

Board of Post Graduate Studies

Department of Chemistry

Sri Venkateswara University

Tirupati-517 502

INORGANIC CHEMISTRY - I
PAPER - CHEM 701C

Total Marks: 100 (Theory 80 + Internal Assessment 20)

Credit: 04

Group-A (Credit: 02)

Unit-I Symmetry and Application of Group Theory:

(a) Symmetry elements and operations, equivalent symmetry elements and equivalent atoms, point groups with examples, Group of very high symmetry, systematic procedures for symmetry classification of molecules and illustrative examples, molecular symmetry for compounds having coordination number 2 to 9, molecular dissymetry and optical activity.

(b) Elementary idea of representation of theory, brief review of matrix, representation of groups, reducible and irreducible representation of point groups, definition of classes and character, the "Great Orthogonality Theorem" and its consequences, Orthogonality theorem for character tables, concept of character projection operator. Utilization of symmetry and group theory in constructing MO diagrams for polyatomic molecules (AB_n), the normal mode of vibration, symmetry of normal vibration, selection rules for IR and Raman Transitions, Electronic spectra of some diatomic molecules, selection rules, σ, π and n transitions in Transition metal complexes.

Unit-II Stereochemistry and Bonding:

(a) VSEPR Theory; VBT (diatomic molecule, H_2); Polyatomic molecules; hypervalence; localized bond, hybridization and energetics of hybridization; dπ-pπ bond; Bent's rule; Walsh Diagrams; MOT (simple LCAO); σ, π, δ M.O.; bonding and antibonding M.O. orbitals; criteria for stable molecular orbitals; orbital symmetry and overlap; homonuclear diatomic molecules (H_2^+, H_2); heteronuclear diatomic molecule; polyatomic molecules; molecular shapes in terms of molecular orbitals; Hückel theory (simple treatment);

(b) Structure and bond properties; bond length, bond strength, electronegativity, group electronegativity, bond enthalpy, bond polarity, weak interactions:- hydrogen bonding, π-π stacking, CH-π interaction; metallic bonding:- band Theory, bonding in alloys, intermetallic compounds.

Group-B (Credit: 02)

Unit-III Coordination Chemistry

Brief review of theories of coordination compounds (VBT, CFT), Ligand Field Theory (LFT), Experimental evidences for metal-ligand orbital overlap, Calculation of ligand field parameters for complexes, MO Theory (LCAO) for complexes, application of MOT to octahedral, tetrahedral and square planar complexes, π-bonding in octahedral complexes and its effect on energy of molecular orbitals.

Unit-IV Magneto-chemistry

Brief review (of different types of magnetic behaviour of materials and their origin, magnetic susceptibility and magnetic moment, measurement of magnetic susceptibility Gouy and Faraday methods), quenching of orbital moments, Interpretation of magnetic moments of complexes on the basis of various theories of complexes.

Magnetic behaviour of multi-electron system, orbital coupling, spin-coupling, spin-orbit coupling (Russel Saunder's coupling), spin-orbit coupling constant, spin-orbit interaction energy, j-j coupling, micro-states and term symbols, Hund's rule for ground state term symbol, Lande interval rule, Derivation of Curie equation for magnetic moment, Curie and Curie-Weiss law, Thermal energy and magnetic moment, antiferromagnetism and its exchanged pathways.

Text Books

1. J. E. Huheey, E. A. Keiter, R. L Keiter and O. K. Medhi. Principles of Structure and Reactivity. First impression, Pearson Education 2006.
2. F. A. Cotton. Chemical Applications of Group Theory (3rd Edn) John-Wiley and Sons (1990)
3. F. A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry (4th and 5th edition) John Wiley (1988)
4. R. L. Dutta & A. Syamal, Elements of Magnetochemistry.
5. W. L. Jolly, Modern Inorganic Chemistry.
6. Gary L. Miessler and Donald A. Tarr, Inorganic Chemistry (4th Edition)
7. David M. Bishop Group Theory and Chemistry (Dover Books on Chemistry)

Reference Books

1. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, Shriver and Atkins Inorganic Chemistry, Oxford University Press (2006).
2. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984).
3. S. F. A. Kettle, Physical Inorganic Chemistry, Spectrum (1996).
4. D. Banerjee, Coordination Chemistry.

ORGANIC CHEMISTRY -I

PAPER: CHEM 702C

Total Marks: 50 (Theory 40 + Internal Assessment 10)

Credit: 02

Unit I: Reaction Mechanism (1 credit)

HSAB principle and its application in organic chemistry; Kinetic and nonkinetic methods for determination of reaction mechanisms; Linear free energy relationship; the Hammett equation-substitution and reaction constants; Taft treatment of polar and steric effects in aliphatic compounds; addition reactions of allenes and carbonyl compounds, stereochemistry of substitution, addition and elimination reactions; Substitution vs elimination reactions; aromaticity and antiaromaticity; aromatic ions.

Unit II: Advanced Stereochemistry (1 credit)

Symmetry elements and point groups, axial and planar chirality, correlation of axial dissymmetry and Centro dissymmetry, atropisomerism, stereochemistry of allenes, biphenyls and spirocompounds. Topicity, acyclic systems up to 4 chiral centers, Compounds with asymmetric carbons in branched chains, asymmetric synthesis, Winstein- Holness equation and the Curtin- Hammett principle, conformational analysis of cyclic compounds such as substituted cyclohexanes, fused ring systems (decalinns, PHA, PHP), bridged rings (norborane); allylic strains, alkylketone effects, haloketone rule, trans annular interactions, Concept of ORD, CD, octant rule; asymmetric synthesis.

Recommended text and reference books:

1. F. A. Carey and R. J. Sundberg. Advanced Organic Chemistry. 5th Edn. Plenum

2. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4th edn, John Willey, 1992.

3. D. Nasipuri, Stereochemistry, Conformation and mechanism, 2nd Edn. John Wiley

4. R.T. Morrison and R.N. Boyd, Organic chemistry, 6th edn, Prentice hall of India, New Delhi, 2003.

PHYSICAL CHEMISTRY – I

PAPER: CHEM 703C

Total Marks: 50 (Theory 40 + Internal Assessment 10)

Credit: 02

UNIT –I

QUANTUM MECHANICS–I:

General Principles of Quantum Mechanics

Introduction; linear operators; Hermitian operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; separability of Schrodinger equation ; equation of motion.

Application to Simple Systems and Approximation Methods

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential, tunnelling effect and hydrogen atom. Antisymmetry principle and many–electron wave finctions.

Chemical Binding

Born–Oppenheimer approximation (Introduction); valence bond (VB) and molecular orbital (MO) theory for diatomic molecules – hydrogen molecule ion, hydrogen molecule; excited states of H_2 – singlet and triplet; non–crossing rule and correlation diagram; hybridization

UNIT –II

KINETIC THEORY AND TRANSPORT PROPERTIES OF GASES:

Derivation of Maxwell's distribution of molecular speed; The general equation for transport, Thermal conductivity of gases, Molecular collisions and mean free path, Viscosity of gases, Diffusion , Introduction to the concept of non–steady state, Numerical problems.

CHEMICAL KINETICS–I :

Opposing and consecutive reactions, complex reactions, Atomic and free radical chain reactions. Kinetic salt effect; Effect of solvent on rate constant (Single sphere and double sphere model): Non–Arrhenius equations and its significance. Theory of absolute reaction, rate (statistical) and comparison with that of collision theory; Kinetics of enzyme reaction (effect of pH) Michaels–Menton Law, derivation; Numerical problems

Reference books:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. D. A. MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
3. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, Tata McGraw Hill, 1997.

4. I. Levine, *Quantum Chemistry*, (1994)Tata McGraw Hill, New Delhi.
5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry,* (1935), McGraw Hill, New York.
6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics,* 3rd Ed.(1997) Oxford University Press.
7. K.J.Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
8. H.Eyring, S.H. Lin and S.M.Lin, *Chemical Kinetics*, (1999)Jhon Willey, New York.

CHEMISTRY PRACTICAL-I

Paper: CHEM 704C

Credit: 04

Group A: Laboratory Course in Inorganic Chemistry

Semi micro qualitative analysis of Inorganic salt mixtures containing (06) six radicals including W, Mo, V, Ti, U, Th, Zr, Ce and at least one interfering radical ($F^-/PO_4^{3-}/BO_3^{3-}$).

Group B: Laboratory Course in Organic Chemistry

Separation, purification and identification of compounds of binary solid mixtures by systematic analysis

Group C: **Laboratory Course in Physical Chemistry**

Quantitative analysis:

1. Determination of specific rotation of cane sugar and determination of concentration of supplied sample.(Quantitative-one day).
2. Potentiometric titration of Co(II) by $K_3[Fe(CN)_6]$ and determination of concentration of Co(II) in a solution. (Quantitative-one day).
3. Conductomectric titration of triple mixture containing KCl, NH_4Cl and HCl by $AgNO_3$ and by NaOH solution. (Quantitative-one day).
4. Verification of Beer's law and determination of concentration of unknown solution spectrophotmetrically(Quantitative-one day).
5. Determination of strengths of halides in a mixure , potentiometrically.
6. Determination of pH of buffer solutions and hence to calculate the E0 of quinhydrone electrode
7. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
8. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.

DEPARTMENT OF CHEMISTRY
TRIPURA UNIVERSITY
(A CENTRAL UNIVERSITY)
(Syllabus-2015)

Choice Based Credit system (CBCS)

Semester – II

CORE

CHEM	801C	Inorganic Chemistry-II	02
CHEM	802C	Organic Chemistry-II	04
CHEM	803C	Physical Chemistry-II	02
CHEM	804C	Chemistry Practical-II	04

ELECTIVE

CHEM	805E	Spectroscopic methods in inorganic Chemistry	02
CHEM	806E	Nuclear and Radiation Chemistry	02
CHEM	807E	X-ray Crystallography	02
CHEM	808E	Pericyclic and Organic Photo Chemistry	02
CHEM	809E	Chemistry of Bio Molecules	02
CHEM	810E	Medicinal Chemistry-I	02
CHEM	811E	Irreversible Thermodynamics and Non-Equilibrium Thermodynamics	02
CHEM	812E	Spectroscopy-II	02
CHEM	813E	Polymer chemistry	02

INORGANIC CHEMISTRY – II
PAPER – CHEM 801C

Total Marks: 100 (Theory 35 + Internal Assessment 15)

Credit: 02

Unit I: Kinetics and Mechanism of Inorganic Reactions

(a) Labile and inert complexes, mechanisms of ligand substitution reactions, ligand substitution reactions in square planar and octahedral complexes, the trans effect, mechanism of isomerization reaction, Linkage isomerism, cis-trans isomerism, intra- and intermolecular racemization of tris-chelate complexes, Ray-Dutta and Bailar twist mechanisms.

(b) Mechanism of electron transfer (redox) reactions: various types of electrons transfer reaction (inner and outer sphere reactions, complementary and non-complementary reactions, self-exchange reactions), Marcus-Husch theory and its applications, correlation between thermal and optical electron transfer reactions, Relation involving structural changes, stereospecific reaction, stereochemical non-rigidity and fluxional molecules.

Unit II: Study of complexes in solution

Stability of a complex in solution, thermodynamic and kinetic stability of complexes, factors affecting thermodynamic and kinetic stability of complexes, stability constant, determination of composition and stability constants of complexes by modern methods, conditional stability constants and their importance. Study of polynuclear and mixed ligand complexes.

Unit III: Transition and Inner transition metal chemistry

(a) Chemistry of Platinum metals: Important compounds of Platinum metals, comparative study of Lanthanides and Actinides with reference to oxidation states, complex formation, magnetic properties, colour and spectral properties, Lanthanide shift reagents.

(b) Transition metal π-acid complexes: π-acid ligands (CO, NO, tertiary phosphine, arsine etc.), structure, bonding, synthesis and reactivity of complexes of CO, NO, tertiary phosphine, metal carbonyl hydrides.

ORGANIC CHEMISTRY – II
PAPER – CHEM 802C

Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 04

Group A

Unit I Reactive Intermediates (1 credit)

a) Arynes: Generation, structure and stability; Benzyne mechanism for aromatic nucleophilic substitution; Rearrangement and cyclo-addition reactions of arynes.
b) Enamines: Generation, structure and stability of enamines; synthetic applications.
c) Free radicals: Generation, structure and stability of radicals, substitution and addition reactions involving radicals, radical- initiator, scavenger, oxidative stress induced free radicals, brief idea about post translational modification of proteins (oxidation, nitration) and DNA scission.

Unit II Reagents in Organic Synthesis (1 credit)

Uses of the following reagents/reactions in organic synthesis: PCC, PDC and Collin's reagent; IBX, Dess-Martin periodinane, ceric ammonium nitrate, Thallium(III) nitrate, chloranil, DDQ, m-CPBA, K-selecteride and L-selecteride, sodium cyanoborohydride, super hydrides, 9-BBN, Mukaiyama reagent, Gilman's reagent, LDA, dicyclohexylcarbodimide, trimethysilyl iodide, tri-n-butyltin hydride, NCS, NBS, NIS, Corey-Nicolaou reagent, baker's yeast, CBS reagents, diimide, crown ether, phase transfer catalyst.

Group B

Unit III: Strategies in organic synthesis (1 credit)

Retrosynthetic analysis, Designing of organic synthesis with special emphasis on disconnection approach; Reversal of dipoles (umpolung of reactivity) and it's applications; Synthons and retrons, linear and convergent synthesis, protection and deprotection strategies, protecting agents for common functional groups; Trans metallation approach and metal catalyzed cross coupling reactions.

Unit IV: Selective named reactions (1 credit)

Arndt Eistert synthesis, Swern oxidation, Moffat oxidation, Prevost and Woodward hydroxylation; Henry reaction, Wittig reaction and Horner-Wordwoth-Emmons reaction (stabilized and non-stabilized ylide); Nazarov cyclization, Pictet-Sprengler reaction, Biginelli reaction, Passerini reaction, Ugi reaction, Peterson's synthesis, McMurry olefination, Julia olefination, Tebbe Olefination. Shapiro reaction, Chichibabin reaction, Baeyer-Villiger oxidation, Baylis-Hillman Reaction, Dienone-Phenol Rearrangement, Staudinger Reaction, Stobbe Condensation.

Recommended text and reference books:

1. W. Carruthers. *Some Modern Methods of Organic Synthesis* (4th edn.), Cambridge University Press (2004).

2. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry, 3rd Edition (2002), McMillan
3. L. Stryer, Biochemistry, 5th Edition (2002), Freeman & Co, New York.
4. H. O. House, Modern Synthetic Reactions, 3rd Edition (1992), Benjamin Publishing Co.
5. S. Warren, Organic Synthesis, Disconnection Approach, 1982, Wiley Interscience, New York.
6. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry Part A and Part B, 5th edition (2007), Springer.
7. Michael B. Smith & Jerry March, Advanced Organic Chemistry Reactions, Mechanisms, and Structure. (2013) Wiley-Interscience
8. T. Laue and A. Plagens, Named Organic Reactions, 2nd edition (2005), John Wiley & Sons Ltd
9. *Reinhard Bruckner* Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
10. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press.

PHYSICAL CHEMISTRY – II
PAPER - CHEM 803C

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credit: 02

UNIT-I: CHEMICAL THERMODYNAMICS

Nernst heat theorem and the third law of thermodynamics, Calculation of entropy changes in chemical reactions, Mathematical and thermodynamic probability. Entropy and probability. The free energy of a mixture. Dependence of thermodynamic functions on composition. Partial molar quantities.

Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures. Concept of fugacity.

Analytical form of the chemical potential in ideal solutions. Chemical potential of the solute in a binary solution Application of Gibbs-Duhem equation.

The concept of activity:the rational concept and the practical concept. Colligative properties and activity of solute. Activities and reaction equilibria, experimental determination of activity coefficients of non-electrolytes, Numerical problems.

UNIT-II: SPECTROSCOPY-I

Rotational (microwave) spectra, rigid diatomic molecule, Energy expression; Rotational constant. Selection rules. Determination of bond length from observed rotational spectra. Spectral intensity-degeneracy of rotational energy levels and total relative population. The effect of isotopic substitution. Non-rigid rotator (energy expression only).Chemical analysis by microwave spectroscopy.

Vibrational (infra-red) spectra:Simple harmonic oscillator model. Corresponding selection rule. Anharmonic oscillator model-Morse function. Selection rules. Fundamental absorption and overtones. Hot bands. P-,Q-,R- branch in IR spectra. Frank-Condon principle. IR spectra of linear molecules. Parallel and perpendicular vibrations. Chemical analysis by IR techniques.

Raman spectroscopy: Rayleigh scattering and Raman scattering (classical and quantum mechanical consideration). Stokes and Anti-stokes lines. Selection rule. O- and S-branch in Raman spectra. Rotational Raman spectra of homonuclear diatomic molecules. Vibrational Raman Spectra .The rule of mutual exclusion. Structure determination from Raman and IR spectra.

Numerical problems.

Reference books:

1. G. W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. P. W. Atkins, *Physical Chemistry*, 7th Ed.(2002) Oxford University Press, New York.
3. K. Zeemanski, *Thermodynamics*
4. C. N. Banwell and E. M. Mc Cash, *Fundamentals of Molecular Spectroscopy*, 4th Ed. (1994) Tata McGraw Hill, New Delhi.
5. G. Herzburg, *Infrared and Raman Spectroscopy*,(1945), *Spectra of Diatomic Molecules* (1950), Van Nostand, New York Addition Wesley, Longman Ltd.
6. Raymond Chang, *Basic Principle of Spectroscopy*, (1971) McGraw Hill.
7. G. M. Barrow, *Introduction to Molecular Spectroscopy*,
8. G. M. Hollas, *Modern Spectroscopy*, (1976) John Willey, New York.

CHEMISTRY PRACTICAL-II

PAPER: CHEM 804C

Credit: 04

Group A: Laboratory Course in Organic Chemistry

1. Identification of organic liquid compounds by systematic analysis
2. Organic preparation
3. Organic estimation - Estimation of glycine by Sorensen's formal titration

Group B: Laboratory Course in Inorganic Chemistry

Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three component mixtures and alloys.

Group C: Laboratory Course in Physical Chemistry

1. Determination of rate constant and order of the reaction between $KBrO_3$ and KI in acid medium.(Qualitative- one day)
2. Kinetic study of decomposition of $K_2S_2O_8$ by KI and effect of added salt. (Qualitative- two day)
3. Determination of formula of cupro-ammonium ion. (Qualitative- one day)
4. Determination of distribution coefficient of C_6H_5COOH between H_2O and an organic solvent (verification of dimerization of benzoic acid in organic solvent). Qualitative-one day)
5. Determination of standard electrode potential of quinhydrone electrode. (Qualitative-one day).
6. Determination of composition and stability constant of Ferric-salicylic acid complex by Job's method. (Qualitative-two day).
7. Determination of critical micellar concentration(CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.

Reference books:

1. N. K. Visnoi…..
2. D. P. Shoemaker, C. W. Garland and J. W. Niber, *Experiments in Physical Chemistry*,(1996) McGraw Hill Interscience.

3. Findlay's Practical Physical Chemistry, 9th Ed. Revised by B.P. Levitt, Longman.1973.
4. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
5. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).
6. A. I. Vogel. *Practical Organic Chemistry* (3rd edn.), Longman Group Ltd. (1973).

PAPER – CHEM 805E

(Spectroscopic methods in inorganic Chemistry)
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit I:

Nuclear Magnetic Resonance Spectroscopy:

General principle, Larmor precession, condition for magnetic resonance, Relaxation time-spin lattice and spin–spin relaxation, Chemical shift and its measurement, various factors that contribute to chemical shift (ring currents, magnetic anisotropy), shielding and de-shielding mechanism. Use of chemical shifts and spin-spin couplings for structural determination. Application of ^{1}H, ^{13}C, ^{19}F and ^{31}P spectroscopy in the structural assignment of inorganic compounds.

Electron Spin Resonance Spectroscopy:

Basic principle, Hyperfine splitting (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero – field splitting and Kramers degeneracy); Anisotropic effects (the g-value and the hyperfine couplings). Application of ESR- ESR spectra of simple free radicals, ESR spectra of transition metal complexes (d^1 and d^9 ions in cubic and tetrahedral fields),anisotropic nature of g-values, metal hyperfine coupling constant, ESR spectra in structural assessment of inorganic compounds.

Unit II :

Infrared and Raman Spectroscopy:

Comparison of IR and Raman spectroscopy; application of vibrational spectroscopy in investigating - Symmetry and shapes of simple AB_2, AB_3 and AB_4 molecules on the basis of spectral data.

Structural elucidation of co-ordination compounds containing the common ligands such as: NH_3, H_2O, OH^-, $NO3^-$, $SO42^-$, ClO_4^-, CN^-, N_3^-, H^-, PR_3, OPR_3, halides, dioxygen, $-COO^-$.

Mass Spectroscopy:

Basic principle of mass spectrometry, concept of metastable ions and transitions, recognition of the molecular ion peak, Stevensan's rule, basic differences in fragmentation of and bonded metal compounds.

Application to metal compounds containing ligand such as carbonyl/ nitrosyl/ alkyl/ cyclopentadienyl and acetyl acetonate. Interpretation of mass spectra for structural characterization. Effect of isotopes on the appearance of mass spectrum.

Recommended Books:

1. R.S. Drago, Physical Methods for Chemists(1992), Saunders College Publishing, Philadelphia.
2. K. Nakamoto, Infrared Spectra of Inorganic and coordination compounds, 2nd Edn. 1970, Wiley-Interscience, London.
3. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication (Zeneca) 1997).

PAPER – CHEM 806E

(Nuclear and Radiation Chemistry)

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credit: 02

Unit I: Nuclear and Radiation Chemistry **15 lecture**

Nucleus and its elementary particles (nucleons and subnucleons), classification of nuclides, nuclear stability and its factors, Binding Energy (BE) of nuclide, BE and Mass systematics, Nucleus is a storehouse of atomic energy, Nuclear reactions and Bethe's notation, Types of nuclear reactions, Nuclear reaction energetics, Nuclear fission and nuclear fusion reactions are ultimate source of energy, fission product and fusion yields, mass and charge distribution in fission, fusion cross section, Nuclear fusion and steller energy.

Nuclear modes: Shell model, Liquid drop model, Fermi gas model, Collective model, Optical model.

Concept of nuclear reactors and moderators for fission reaction, Nuclear waste management.

Unit II: Elements of Radiation Chemistry:

Interaction of ionising radiation with matter, units for measuring radiation absorption and radiation energy, radiation dosimetry, radiolysis of water and aqueous solutions.

Applications of radioisotopes - General principles of using radioisotopes, applications of radiotracers in-

a) Physicochemical constants - diffusion coefficient, surface area, solubility, stability constant.
b) Chemical pathways - kinetic studies, inorganic reactions, organic reaction, biosynthesis, polymerization.
c) Trace analysis of elements and compounds - neutron activation analysis, isotope dilution analysis.

Text Books

1. Essentials of Nuclear Chemistry, H. J. Arnikar, 4th Edition Wiley Eastern (1987).
2. Introduction of Nuclear and Radiochemistry, G Friedlander, T. W. Kennedy, E. S. Macias and J. M. Miller, 3rd Edition, John Wiley (1981).

PAPER: CHEM 807E

X-ray Crystallography

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I

Crystals Lattices and symmetry: Definition of a crystal, Lattice points, Unit Cells, Unit Cell calculations; Definition of symmetry, Symmetry operations and elements of symmetry, Point groups, Classification of unit cells, Crystal systems, Herman-Mauguin notation, Bravais Lattices, Distinction between trigonal and hexagonal systems, Crystal planes and indices Law of rational indices.

Space groups and equivalent positions: Screw axis, Glide planes, Space groups, Relationship between space groups, point groups, and physical properties, Equivalent positions, Special positions, Space group tables in International Tables for X-ray crystallography.

Unit III

X-ray diffraction: Periodicity and structural information, The diffraction grating, Diffraction of X-ray by crystals, The Laue equations, Bragg's Law, Generalization of Miller indices, Electron density function, Fourier series, Fourier expansion of electron density, Intensities of diffraction spots, The phase problem, Calculation of structure factors, Effect of thermal vibrations, Structure factors of centro-symmetric crystals, Friedel's law, Laue groups, Structure factors of sodium chloride

Determination of atomic positions: Solutions of structure factor equations, The Patterson function Heavy-atom methods, Isomorphous replacement, Superposition methods, Inequalities, Sayre-Cochran-Zachariasen relationship, Hauptman-Karle methods, Summary of phase-determining methods, Refinement, Description of procedure for X-ray structure analysis (NaCl and CsCl)

Recommended Books:

1. Introduction to Crystallography, Donald E. Sands, Dover Publications, INC. New York.
2. Crystal Structure Analysis for Chemists and Biologist, Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, Wiley VCH, 1994.
3. Crystal Structure Determination, William Clegg, Oxford University Press, 1998.
4. Structure Determination by X-ray Crystallography, Mark Ladd and Rex Palmer (September 30, 2003).
5. Crystal Structure Determination, Werner Massa (March 31, 2004).
6. Crystal Structure Analysis, Jenny Glusker and Kenneth Trueblood (August 1992).

PAPER: CHEM 808E

Pericyclic and Organic Photochemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit – I: Pericyclic Reactions:

Introduction to pericyclic reactions, orbital symmetry, electrocyclic, cycloaddition, sigmatropic and group transfer reactions; Woodward-Hoffmann rules and orbital motions in different pericyclic reactions. Rationalization based on FMO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. chelatropic reactions. Cope, aza-Cope, oxy-Cope, Claisen and Hoffman-Loefler-Freytag rearrangements, Somelett-Hauser rearrangements.

Unit – II: Organic Photochemistry:

Introduction to organic photochemistry, Frank Condon principles, Jabolonski diagram, photochemical excitation and nomenclature of excited states, Quantum yields, photosensitization and its uses. Photochemistry of olefins and carbonyl compounds, Norrish – I and Norrish – II type reactions, photo oxygenation and photo fragmentation, Paterno-Buchii reaction, Barton reaction, Di-π-methane rearrangement, Photocycloaddition and Photochemistry of arenes.

Recommended text and reference books:

1. F. A. Carey & R. J. Sanburg. *Advanced Organic Chemistry*, Part A and B, 5th Edn. (1990).
2. J Singh. Organic Photochemistry and Pericyclic reaction.
3. C. Depuy & O. L. Chapman. *Molecular Reactions and Photochemistry*, Prentice-Hall of India (1975).

4. R. B Woodward & R. Hoffman, *Conservation of Orbital Symmetry*; Verlag-Chemie/ Academic Press (1970).
5. I. Fleming. *Frontier Orbital Theory and Organic Reactions*, John Wiley & Sons (1976).
6. A. P. Marchand & R. E. Lehr, *Pericyclic Reactions*, Academic Press (1977).
7. John D. Coyle, Introduction to Organic Photochemistry (1989), John Wiley and Sons.

PAPER - CHEM 809E

Chemistry of Biomolecules

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I:

Chemistry of amino acids and peptides: Structures, properties and synthesis of amino acids; essential amino acids; nomenclature and sequencing of polypeptides; polypeptide synthesis via solution and solid phase methods; structures of proteins; protein denaturation; biosynthesis of amino acids and proteins.

Unit II:

Chemistry of carbohydrates and lipids: Classification; structure, stereochemistry, conformation, some reactions of mono and disaccharides; carbohydrate metabolism; role of sugars in biological recognition.

Classification of lipids, Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, biological membranes, lipid peroxidation, properties and function of lipid bilayers and liposomes; self association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.

Recommended text and reference books:

1. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford.
2. G. C. Barrett and D. T. Elmore, Amino acids and peptides (2004), Cambridge University press.
3. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
4. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
5. Organic Chemistry, McMurry
6. Organic Chemistry, Bruice
7. *Norbert Sewald and Hans-Dieter Jakubke,* Peptides: Chemistry and Biology.. Wiley-VCH
8. Ward, Selectivity in organic synthesis (1999), Wiley-VCH, 1999.
9. T. W. Greene, Protecting groups in Organic synthesis (2000), Wiley-VCH, 2000.

PAPER - CHEM 810E

Medicinal Chemistry-I

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I:

Drugs and drug design: Concepts of drugs, classification, analogues and pro-drugs, theories of action, assay and metabolism of drugs;

Drug design, theory of drug design, structure activity relationship (SAR), introduction to combinatorial synthesis in drug discovery; Development of new drugs, procedures followed in drug design, Quantitative structure activity relationship (QSAR); History and development of QSAR.

Unit II:

Synthesis and uses of the following drugs of different pharmacological activities:

a) Antibiotics: Preparation of semi synthetic penicillin, conversion of penicillin into cephalosporin, synthesis of chloramphenicol (diastereoselective and enantioselective) general account of tetracycline & macrocyclic antibiotics (no synthesis)

b) Antimalerials: Trimethoprim

c) Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.

d) Anti- inflammatory: Ibuprofen, Oxyphenylbutazone, Diclophenac, Indomethacin.

e) Antitubercular&antileprotic: Ethambutol, Isoniazide&Dapsone

f) Anaesthetics: Lidocaine, Thiopental.

g) Antihistamines: Phenobarbital, Diphenylhydramine.

h) Tranquilizers: Diazepam, Trimeprazine.
i) Anti AIDS: General study
j) Cardiovascular: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol
k)Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloraethamine, cyclophosphamide, Mephalan, uracils, mustards.

Recommended text and reference books:

1 A. Kar, Medicinal Chemistry, New Age publications
2 Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-*A Molecular and Biochemical Approach*, Oxford University Press.
3 Burger. *Medicinal Chemistry and Drug Discovery*, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
4 Goodman & Gilman. *Pharmacological Basis of Therapeutics*, McGraw-Hill (2005).
5 S. S. Pandeya & J. R. Dimmock.*Introduction to Drug Design*, New Age International.(2000).
6 D. Lednicer. *Strategies for Organic Drug Synthesis and Design*, John Wiley (1998).
7 Graham & Patrick. *Introduction to Medicinal Chemistry* (3rd edn.), OUP (2005).

PAPER – CHEM 811E

Irreversible Thermodynamics and Non-Equilibrium Thermodynamics

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

IRREVERSIBLE THERMODYNAMICS:

Entropy of irreversible processes – Clausius inequality; entropy production and entropy flow, Rate of entropy production – generalized forces and fluxes (heat flow, chemical reactions, electrochemical reactions); Entropy production in open system; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; Stationary non-equilibrium states -states of minimum entropy production.

UNIT II

NON EQUILIBRIUM THERMODYNAMICS

Non-equilibrium statistical mechanics: Random Processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.

Reference books:

1. C. Kalidas and M.V.Sanganarayana, Non Equilibrium Thermodynamics – Principles and application, Macmillan India (2002).
2. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Interscience (1960).

PAPER – CHEM 812E

SPECTROSCOPY -II

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

NMR: Theory for ^{1}H NMR Population of energy levels. Larmor precession. Relaxation times: spin - lattice relaxation, spin-spin relaxation. Fourier transform spectroscopy in NMR . Chemical shift. Shielding and de-slielding mechanism. Fine structure, spin-spin splitting, coupling constant. Strongly coupled systems, shift reagent in NMR. Hyperfine structure. Nuclear overhauser effect (NOE), 1H and ^{13}C NMR. Two-Dimentional NMR. Chemical analysis by NMR techniques.

ESR : General background of ESR spectroscopy .Representation of ESR spectrum. 'g' - value, ESR spectra of simple organic free radicals; Hyperfine coupling, prediction of expected number of lines and their relative intensities, ESR spectra of transition metal complexes, metal- hyperfine coupling, anisotropic ESR spectra, zero field splitting, application of ESR spectroscopy examples.

UNIT-II

***Photoelectron Spectroscopy (PES)* :** Basic principles of photoelectron and X-ray photoelectron spectroscopies and their applications for chemical analysis of surfaces; application of ESCA and Auger spectroscopy for the studies of solids.

NQR: Nuclear quadruple resonanse, Energy levels of a nucleus in a non-uniform electric field. Quadruple coupling constant. NQR spectra of molecular compounds.

Mossbauer Spectroscopy: Principles of Mossbauer spectroscopy, Doppler shift, emitted quantum, Mossbauer spectra and chemical structure.

Reference books:

1. C. N. Banwell and E.M. Mc Cash, *Fundamentals of Molecular Spectroscopy,* 4th Ed. (1994) Tata McGraw Hill, New Delhi.
2. G. Herzburg, *Infrared and Raman Spectroscopy*,(1945), *Spectra of Diatomic Molecules* (1950), Van Nostand, New YorkAddition Wesley, Longman Ltd
3. Raymond Chang, *Basic Principle of Spectroscopy*, (1971) McGraw Hill.
4. G. M. Barrow, *Introduction to Molecular Spectroscopy,*
5. G. M. Hollas, *Modern Spectroscopy,* (1976) Jhon Willey, New York.

PAPER – CHEM 813E
POLYMER CHEMISTRY
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

UNIT-I:

Polymer and Characterisation:-Banz concepts of polymer science, Molecular forces and chemical bonding in polymers.Polymer solution and fractionation. Gel permeation, Chromatography and molecular weight determination by viscometry, osmometry, light scattering and ultra centrifugation, molecular weight distribution curve.

UNIT-II:

Polymerization :- mechanism and kinetics of step growth and chain growth polymerization-radical, ionic and ring opening polymerization, copolymerization, polymerization techniques and polymer reaction, polymer structure and physical properties: configuration of polymer chain crystal structure of polymers: speciality polymers: Block copolymer, polymer colloids and biomedical polymers.

Reference books:

1. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
2. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
3. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
4. G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
5. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
6. F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New York.

SEMESTER – III

Semester - III

CHEM 901C	Inorganic Chemistry-III	02
CHEM 902C	Organic Chemistry-III	02
CHEM 903C	Physical Chemistry-III	04
CHEM 904C	Chemistry Project-I	04

Elective

CHEM 905E	Metal Clusters	02
CHEM 906E	Inorganic Polymers	02
CHEM 907E	Analytical Techniques in Chemistry	02
CHEM 908E	Chemistry of Macromolecules	02
CHEM 909E	Chromatographic Techniques	02
CHEM 910E	Enzyme Chemistry	02
CHEM 911E	Surface Chemistry	02
CHEM 912E	Statistical Thermodynamics	02
CHEM 913E	Advanced Group theory	02

INORGANIC CHEMISTRY – III

PAPER – CHEM 901C

Credit: 02

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Unit I: Electronic Spectra of Transition metal complexes:

Spectroscopic states: micro states, terms of d^n configurations, Selection rules, Orgel diagram, Correlation diagram, Tanabe-Sugano diagram, calculation of ligand field parameters (dq, B and β values), Band intensities and band width, Spectra of high spin octahedral and tetrahedral complexes for d^1-d^9 systems, charge transfer spectra, Application of electronic spectra for structural characterization of coordination compounds.

Unit II: Organometallic Chemistry:

Introduction: Definition, a brief history of organometallic chemistry, importance of organometallic compounds as reagents, additive and catalyst.

Fundamentals of Organometallic chemistry: Application of 18 and 16 electron rule to transition metal organometallic complexes, Counting of electrons and finding metal-metal bond.

Transition metal organometallic compounds containing metal-carbon σ –bonds: Synthesis, reactivity and structural aspects of sigma alkyls, mixed alkyls, alkylate ions, chelate alkyls, metal carbene (CR_2 bridges) and carbyne (CR-bridges)

Transition metal organometallic compounds containing metal-carbon π -bonds: Synthesis, Structure and bonding of transition metal complexes with olefins, cyclopentadienyl, cyclopentadienide and benzoid systems. Allyl and other enyl complexes, complexes containing 3 or 4 member rings, metal compounds of heterocycles, multidecker sandwich compounds.

Recommended Books:-

1. J. Huhee, E.A. Keiter, R.L. Keiter & O.K. Medhi-Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn..Pearson Education, 2007.
2. G.L. Miessler & D.A. Tarr-Inorganic Chemistry, 3rd Edn, Pearson Education, 2007.
3. Allan K. Brisdon-Inorganic Spectroscopic methods, Oxford.
4. Introduction to Ligand field Theory- B.N.Figgis
5. Basic Organometallic Chemistry - Concepts, Syntheses and Applications by B. D. Gupta, A. J. Elias, Universities Press (2010).
6. Organometallic Chemistry: A Unified Approach by R. C. Mehrotra, Anirudh Singh, 2nd Edition, New Age International, Publication Year: 1991, reprint (2014).

ORGANIC CHEMISTRY-III
PAPER-CHEM 902C
Credit: 02
Total Marks: 50 (Theory 35 + Internal Assessment 15)

Unit I: Proton magnetic resonance spectroscopy (No. of lectures 18)

Introduction – spin active nuclei, Continuous wave (CW), Fourier transform (FT) NMR spectrometer, Phenomenon of resonance and relaxation, instrumentation and sample handling, chemical shift, internal standards, factors affecting the chemical shift, NMR shift reagents, shielding and deshielding of a nucleus, empirical co-relations for proton chemical shifts, anisotropic effect, effect of solvents, effect of hydrogen bonding, influence of chirality, spin-spin coupling – vicinal and geminal coupling, long range coupling – two bond coupling ($_2J$) three bond coupling ($_3J$), Karplus relationship, multiplicity of splitting and relative intensity of lines, spin decoupling, coupling constants. First order spectra- A_3X, AX and AMX systems. Second order spectra- AB and A_2B_2 systems.

Unit II: Mass spectroscopy **(No. of lectures 12)**

Introduction – basic theory, instrumentation and sample handling. Methods of generation of mass ions – electron impact (EI), chemical ionization (CI), electron spray ionization (ESI) and fast atom bombardment (FAB) techniques, TOF-MALDI and SELDI; Tandem mass spectroscopy, general mass fragmentation pattern of organic compounds, base peak, molecular ion, relative intensity, mass ions fragmentation, metastable ions, even electron rule, nitrogen rule, HDI, application of mass spectroscopy, Characteristic fragmentation pattern of organic compounds.

Recommended books:

1. Spectroscopic identification of organic compounds (8th edition). R.M. Silverstein and F.X. Webster, John Wiley & Sons, Inc (2014).
2. Spectroscopic methods in organic chemistry (sixth edition). D. H. Williams and I Fleming, Tata McGraw Hill (2005).
3. Organic spectroscopy (3rd edition). William Kemp, MacMillan (1991).
4. Applications of Absorption Spectroscopy of Organic Compounds. J.R. Dyer. Prentice Hall (Digitized 2008)
5. Introduction to Spectroscopy (5th Edn), Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan (2009)
6. Spectroscopic problems in organic chemistry (5th Edn.), Williams and Flemings, Tata McGraw Hill (2007).
7. Organic Spectroscopy-Principles and Applications (2nd Edn), Jagmohan, Alpha Science International Ltd (2004).

PHYSICAL CHEMISTRY-III
PAPER-CHEM 903C
Credit: 04
Total Marks: 100 (Theory 70 + Internal Assessment 30)

Group A: QUANTUM MECHANICS

UNIT-I

Interpretation of wave function (probability density). Box normalization. Superposition principle and expansion theorem. Derivation of the expression of in polar coordinate system. , , and operators are Hermitian : Proof. Unitary and projection operators. Some important theorems. Schmidt orthogonalization. Dynamical variables and operators, dynamical states. Expectation value and average value. Linear vector spaces in quantum mechanics. Completeness theorem. Equations of motion of classical mechanics (in brief). Poisson bracket and Dirac's version of Correspondence principle. Ehrenfest theorem. Constants of motion.

The Heisenberg Uncertainty relations (position and momentum, angle and angular momentum , time and energy relations) : proof. Commutability and compatibility. Complete set of commuting operators. Fourier transform. Wave packet. Momentum space wave function.

Angular momentum operators (single particle system). Step up and step down operators. Spin angular momentum operators. Angular momentum operators (many electron system) and their commutation with spin free Hamiltonian operator. coupling of angular momenta, L-S coupling and j-j coupling. Term symbols and spectroscopic states. Pauli spin matrices and anti-commutation relations.

UNIT-II

Time independent non-degenerate perturbation theory (RSPT). Application: ground state of He atom. Degenerate RSPT. Applications: Stark effect, normal and anomalous Zeeman effect.

Rayleigh- Ritz variation principle. Linear variation method. Applications: ground state energy of He atom, harmonic oscillator.

Time dependent RSPT (First order). Fermi-Golden rule. Born-Oppenheimer approximation(in detail). Antisymmetrized wave Function. Slater determinant and Pauli exclusion principle.

Group B: ADSORPTION & AGGREGATION AND SOLID STATE CHEMISTRY

UNIT –III: ADSORPTION AND AGGREGATION

Surface tension and Surface free energy. Bubbles and drops, Young -Laplace equation, Kelvin equation. Surface thermodynamics. Gibbs adsorption isotherm. Surface films. The B.E.T adsorption isotherm. Estimation of surface area of solids (BET method).Capillary condensation and adsorption hysteresis.

Catalytic activity at surface, electrochemical phenomena at interfaces. The electrical double layer.

Surface active agents and their classification, micellization-hydrophobic interactions, critical micelle concentration (CMC),factors effecting the CMC of surfactants. Thermodynamics of micelle formation-phase separation and mass action models, solubilization, Structure of micelles and reverse micelles, counter-ion binding to micelles.

Emulsion- formation of emulsions, factors determining emulsion stability, microemulsion, foams.

UNIT – IV: **SOLID STATE CHEMISTRY**

Solid State Reactions: Types; sintering; nucleation; Factors influencing the reactivity of solids;Precursors to solid state reactions; Tammann and Hedvall mechanism; Wagner's Diffusion theory of reaction; Material transport in solid state reaction—counter diffusion, Kirkendall effect; Huttig's mechanism; Kinetic model: Reaction in powder compact, parabolic rate law, Jander'srate equation.

Crystal Defects: Types of defects, thermodynamics of Schottky and Frenkel defect formation, Kroger-Vink notation for crystal defects Atomic theory of diffusion—self diffusion mechanism.

Reference books:

1. L.I. Schiff, *Quantum Mechanics*, Third Edition, McGRAW-HILL BOOK COMPANY, 1985.
2. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics,* 3rd Ed.(1997) Oxford University Press.
3. B.H. Bransden & C.J. Joachain, *Physics of Atoms and Molecules*, Longmann Scientific and Technical, 1994.
4. B.H. Bransden & C.J. Joachain, *Quantum Mechanics*, Second edition, low price edition, PEARSON Education, First Indian Reprint, 2004.
5. J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesely Publishing Company.
6. Eugene Merzbacher, *Quantum Mechanics*,Wiley International Edition, 1970.
7. R. Stephen Berry, Stuart A. Rice, and John Ross, Physical Chemistry, Second Edition, Oxford University Press, 2000.
8. N.K.Adams, *Physics and Chemistry of Surface.*
9. A.W.Adamson, *Physical Chemistry of surface.*
10. M.J.Rosen, *Surfactants and Interfacial Phenomena*, (1978) John Willey, New York.
11. Y.Moroi, *Micelles: Theatrical and Application Aspects*, (1992) Plenum Press, New York
12. A. R. West. *Solid State Chemistry and its Applications*, John Wiley (1998).
13. N. B. Hannay. *Solid State Chemistry*, Prentice-Hall (1979).
14. D. K. Chakraborty. *Solid State*, New Age International, New Deldi (1996).

CHEMISTRY PROJECT-I
PAPER-CHEM 904C
Credit: 04
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Online course: 25 (20 + 5)
Lab course: 75 (50 + 25)
Experiment: 20
Submission of report and presentation: 30

List of experiments:

Group A

1. Preparation of the following compounds (At least 2) and characterization by IR, UV-Vis, Conductance & magnetic susceptibility measurements.
   (a) Tris (acetyl acetonato)manganese (III)
   (b) Tris (acetyl acetonato)iron (III)
   (c) Linkage isomer of nitro & nitrido pentammine Cobalt (III) Chloride
   (d) Tris (Ethylene diammine) Nickel (II) Chloride. dehydrate
2. Quantitative analysis of metal ions by spectrophotometric method.
3. Determination of composition of Metal-Ligand ratio in complex compound by Job's method.

Group B

4. Synthesis of benzimidazoles/substituted benzimidazole from o-phenylenediamine and
   i) Formic acid
   ii) Acetic acid
   iii) n-Butyric acid
5. Synthesis of 3-acetyl coumarin from salicylaldehyde and ethylacetoacetate.
6. Synthesis of coumarin-3-carboxylic acid from salicylaldehyde
7. Synthesis of 7-hydroxycoumarin -4-acetic acid from resorcinol and ethyl acetoacetate.

Group C

10. Kinetic study of Iodination of Aniline colorimetrically and effect of pH on the rate constant.
11. Determination of equilibrium constant of acid hydrolysis of an ester.
12. Kinetic study of the reaction between $K_2S_2O_8$ and KI and study on the effect of added salt on the rate constant (primary salt effect).

ELECTIVE

Paper –CHEM-905 E (Metal Clusters)
2 credits
Total Marks: 50 (Theory 35 + Internal Assessment 15)

Unit I

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 – Wades rules – Capping rule, Mingo's Rules – 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 $[Ni_5(CO)_{12}]^{2-}$. Carbide Clusters, Cluster having interstitial main group elements. Synthesize of metal carbonyl clusters, Reaction of metal carbonyl clusters.

Unit II

Metal Halide clusters: Major structural types in Dinuclear, Trinuclear, Tetranuclear Metal-Metal systems – Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures, Quadruple bond, Structure and bonding in Octahedral halides of $[Re_2Cl_8]^{2-}$, $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications.

Reference book

1. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5th Edition, Wiley Interscience, N.Y
2. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
3. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
4. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).

Paper –CHEM-906 E (Inorganic Polymers)

Credits- 02

Inorganic polymers:

Classification, types of inorganic polymerization, Comparison with organic polymers, B-O & B-N polymers, Silicones, Coordination polymers, S-N & S-N-F, P-N compounds, Chalcogen cluster - binary and multi component systems, homolytic inorganic systems. Polysiloxanes, polysilanes, polyphosphazenes, polymeric sulfur – synthesis, structure, properties & applications, co-ordination polymers and organometallic polymers. Coordination polymers: Definition, Classification and design strategies, network topologies, supramolecular isomerism, interpretation, porous coordination polymers, properties and applications.

Paper –CHEM-907 E (Analytical Techniques in Chemistry)

2 credits

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Electrochemical Methods

Electrode processes and thermodynamics of cells: Introduction, Electrochemical Cells and reactions, Faradaic and nonfaradaic processes, nonfaradaic processes and the nature of the electrode solution interface, faradaic processes and factors affecting rates of electrode reactions, Basic electrochemical thermodynamics, formal potentials, reference electrodes, Liquid junction potentials.

Currents in Polarography: Charging or condenser current, Migration current, Diffusion current, Ilkovic equation, influence of supporting electrolyte, limiting current measurements.

Potential sweep methods: Introduction, reversible systems peak current and potential, totally irreversible systems peak current and potential, quasi reversible system, cyclic voltammetry.

Flame Atomic Emission and Atomic Absorption Spectroscopy

Flame Atomic Absorption Spectroscopy: Principles of atomic absorption spectroscopy, Radiation sources, Flame and electrothermal atomization, Limitations in atomic absorption, Interferences, Comparison of absorption spectrometry techniques-flame and graphite furnace, Quantitative Analysis, inductively coupled plasma-mass spectroscopy (ICP-MS).

Flame Atomic Emission Spectroscopy: Atomic emission, Principles of flame emission photometry, Limitations of flame emission photometry, Interference, Qualitative Analysis, Quantitative Analysis, Comparison of flame atomic emission

and absorption spectroscopy. Excitation sources in atomic emission spectroscopy, ICP-AES spectroscopy.

Thermo-analytical Techniques

Thermo gravimetric analysis (TGA), differential thermo gravimetric analysis (DTA), differential scanning calorimetry (DSC), Thermometric titration (principle, technique and application)

Reference Books

1. Electrochemical Methods: Fundamentals and Applications by Allen J. Bard & Larry R. Faulkner, 2nd edition, Wiley India, Copyright 2004, reprint (2006).
2. Principles of Polarography by R. C. Kapoor & B. S. Aggarwal, Wiley Eastern Limited, (1991).
3. A Text-book of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, by A.I. Vogel, 3rd Edition, The English language book Society and Longmans, Green & Co Limited, (1956).
4. Atomic Absorption Spectrometry by B. Welz, M. Sperling, 3rd Edition, Wiley-VCH (1999).

Paper CHEM 908E (Chemistry of Macromolecules)

Credit: 02

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Definition, classification – artificial polymer, natural polymer; electrically conducting polymer, fire resistant, liquid crystal polymers, kinetics of polymerization. Molecular mass determination – osmometry, viscometry, diffusion and DLS methods, chain configuration of macromolecules

Natural macromolecules: Proteins, polysaccharides, nucleic acids, purine and pyrimidine bases of nucleic acids, nucleosides and nucleotides, their structures and nomenclature, structures and functions of NADH, NADP and ATP, Structures of RNA and DNA; replication of DNA; base-pairing, double helical structure of DNA.

Recommended books:

1. Lehninger Principals of Biochemistry, (6th edn). D.L. Nelson & M.M. Cox, Freeman publication (2012).
2. Physical Chemistry of Macromolecules (2nd edn), S. F. Fun, John-Wiley (2004)

Paper CHEM 909E (Chromatographic Techniques)
Credit: 02

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Basic concept of chromatographic separation – adsorption and partition chromatography, theory and handling of different chromatographic techniques – column, thin-layer, and paper chromatography.

Modern chromatographic techniques: Gas chromatography: Basic principle, basic equipment; types of column and their selection; detectors (FID, TCD, ECD, NPD); sample separation and applications. High performance liquid chromatography (HPLC): Instrumentation - basic equipment; pumping and injection system, column and its packing, normal and reverse phases; detectors, sample separation and application.

Gel permeable (filtration) chromatography, Size exclusion chromatography, gel electrophoresis

Recommended books:

1. Vogel's Text Book of Quantitative Chemical Analysis (6^{th} Edition), Prentice Hall (2000).
2. Principles and Practice of Modern Chromatographic Methods, (1st Edition), Robards, Jackson & Haddad, Academic press (1994).
3. Chromatographic Methods (5^{th} Edn), A. Braithwaite, J.F. Smith, Kluwar Academic Publisher (2013).

Paper CHEM 910E (Enzyme Chemistry)

Credits: 02

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Introduction - biological catalysis, nomenclature, classification and specificity. Isolation and purification of enzymes. Methods of enzyme assay. Kinetics of enzyme action - Michaelis-Menten equation, different plots for determination of K_m and V_{max} and their physiological significance. Mechanism of enzyme action - two substrate and multi substrate reactions; enzyme regulation and drug design.

Types of enzymes assisted reactions – **o**xidation, reduction, isomerisation, epimerisation, hydrolysis, phosphorylation, acylation, methylation, decarboxylation, dehydration. Enzymatic hydrolysis of peptide (carboxy peptidase, trypsin, chrymotrypsin and Lys C), cofactors, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), Pyridoxal Phosphate (PP), $NADP^+$, FMN, FAD, lipoic acid and vitamin B_{12}.

Recommended books:

1. Lehninger Principals of Biochemistry, 4th Edition. D.L. Nelson & M.M. Cox, Freeman publication (2012)..
2. Introduction to Enzyme and Coenzyme Chemistry (2nd Edition), T D H Bugg, Wiley-Blackwell (2009)
3. Organic Chemistry of Enzyme-Catalyzed Reactions, (2nd Edition), R. B. Silverman, Academic press (2002)
4. Enzyme Kinetics –Principles and methods, H. Bisswanger, Wiley-VCH (2002).
5. Enzyme kinetics-A modern approach, A. G. Marangoni, Wiley-InterScience (2003)

Paper CHEM 911E (Surface Chemistry)
Credits: 02
Total Marks: 50 (Theory 35 + Internal Assessment 15)

ADSORPTION ISOTHERM:

Thermodynamics of adsorption isotherm, Gibbs adsorption isotherm, Adsorption at solid-liquid, liquid-gas, liquid-liquid interfaces, Effect of added electrolyte on the surface excess of ionic surfactants.

MIXED SURFACTANTS:

Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, Rubingh's treatment, Rodenas treatment, conter ion binding in mixed surfactants.

SOLUBILISATION AND EMULSIFICATION:

Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions, reactions in micellar and microemulsion media.

Reference books:

1. N.K.Adams, *Physics and Chemistry of Surface,*
2. A.W.Adamson, *Physical Chemistry of surface,*
3. M.J.Rosen, *Surfactants and Interfacial Phenomena,* (1978) John Willey, New York.
4. Y.Moroi, *Micelles: Theatrical and Application Aspects,* (1992) Plenum Press, New York

Paper 912E (Statistical Thermodynamics)
Credits: 02
Total Marks: 50 (Theory 35 + Internal Assessment 15)

Independent subsystems and distinguishability. Boltzmann distribution (nondegenerate and degenerate cases). Review of partition function: Thermal De Broglie wavelength. Partition functions for electronic, nuclear, rotational and vibrational degrees of freedom. Thermodynamic quantities in terms of partition functions. Entropy of ideal gas. Gibbs paradox. Equilibrium constants (ideal gas reaction) in terms of partition function.

The mathematical proof of the equipartition of energy principle. Specific heats of solids.

Reference books:

1. D. A.McQuarrie, *Statistical Mechanics*, (2003), Viva Books Pvt. Ltd. New Delhi.
2. M. C.Gupta, *The statistical Thermodynamics*,(1990), New Age International (P) Ltd. New Delhi.
3. M. Dole, Introduction to Statistical Thermodynamics

Paper CHEM 913E (Advanced Group Theory)
Credits: 02
Total Marks: 50 (Theory 35 + Internal Assessment 15)

GROUP THEORY – I:

The concept of groups; group multiplication tables and the rearrangement theorem; subgroups, classes and the related theorems; commutative groups (Abelian), cyclic group; isomorphism and homomorphism. Examples.

Molecular point groups (in Brief) , similarity transformation and the invariance of characters of matrices under such transformation, matrix representation of point groups; reducible, irreducible and equivalent and inequivalent representations; the great orthogonality theorem (no derivation) and its corollaries, character tables, construction of character tables in complex cases such as $D_{6h,}$ T_d etc; the group of Schrodinger equation; basis function for irreducible representation "projection" operator; direct product representation .

GROUP THEORY - II (Physical Applications):

Symmetry factoring of secular equations; LCAO -MO ,II bonding and Huckel's theory ;some examples: ethylene ,bengene ,Naphthalein. symmetry based "selection rules" for cyclization reaction (Woodward Hoffmannrule) Hybrid orbital and Molecular orbitals for AB_n -type molecules. Crystal field theory (CFT) Splitting of energy levels, and terms in a chemical environment. Determining the symmetry types of the normal modes;selection rule for fundamental (infra-red and Raman) vibrational transitions. Mutual Exclusion rule.

Reference books:

1. Chemical Application of Group Theory – F.A. Cotton,3rd edition, A Wiley Interscience publication
2. Group Theory and Quantum Mechanics, M.Tinkham, Tata McGraw Hill, publishing Ltd.
3. Group Theory and Chemistry, David M. Bishop, Clarendon Press Oxford.
4. Group Theory and its application to Physical Problem, M. Hamermeah, Dover publication.

CBCS

TRIPURA UNIVERSITY

SEMESTER –IV

Semester – IV

Core

CHEM	1001C	Inorganic Chemistry-IV	02
CHEM	1002C	Organic Chemistry-IV	02
CHEM	1003C	Physical Chemistry-IV	02
CHEM	1004C	Supra-molecular and Nano Chemistry	02
CHEM	1005C	Chemistry Project-II	04

Elective

CHEM	1006E	Organometallics and Catalysis	02
CHEM	1007E	Bio-Inorganic Chemistry	02
CHEM	1008E	Environmental and Green Chemistry	02
CHEM	1009E	Advanced Spectroscopic Techniques	02
CHEM	1010E	Chemistry of Natural Products	02
CHEM	1011E	Medicinal Chemistry-II	02
CHEM	1012E	Photochemistry	02
CHEM	1013E	Fortran and C, C+, C++ Programming	02
CHEM	1014E	Statistical Mechanics	02

PAPER: CHEM 1001C

Inorganic Chemistry-IV

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit –I: (Credit – 01)

1. Catalysis Using Organometallic Compounds: Terminology in catalysis (Turnover, Turnover number, Turnover frequency or turnover rate, mole fraction, eantioselectivity, stereoselectivity, chemoselectivity, regioselectivity); Comparison of Homogenous and Heterogeneous Catalysis; Catalytic Hydrogenation of alkenes and related reactions: Hydrogenation catalysts, Catalytic cycle of Wilkinson's catalyst, Catalytic asymmetric synthesis, the mechanism of asymmetric hydrogenation using a chiral catalyst.
2. Olefin Metathesis: Well-known olefin metathesis catalysts and their properties, synthesis of Grubbs' and Schrock catalysts, Mechanism of olefin metathesis, ring opening metathesis, cross metathesis, ring closing metathesis, ring opening polymerization metathesis, acyclic diene metathesis polymerization, enyne metathesis, comparison of catalysts, application of catalytic olefin metathesis.
3. Palladium catalyzed C–C coupling reactions: The Heek reaction, Suzuki-Miyaura coupling, Sonogashira coupling, Stille coupling, Kumada coupling, Negishi coupling.
4. Olefin polymerization and oligomerisation reactions: The Ziegler-Natta catalyst, site control and chain end control mechanisms, metallocene based catalysts, post metallocenes catalyst.

Unit –II: (Credit – 01)

Bioinorganic Chemistry -1: Essential and trace element in biological system. Structure and function of biological membranes, mechanism of ion transport across membranes; Role of alkali and alkaline earth metals in biology; Crown either complexes of Na and K, Ionophores, Valinomycin, Sodium and Potassium pump; Catalysis of phosphate transfer by Mg^{2+} ion, storage and transport of calcium; Role

of calcium in muscle contraction, blood clotting mechanism, biological calcification; Toxicities of Hg, Cd, Pb, Cr, Be, Se, As, detoxification of metal ions, Chelation therapy, metals need for diagnosis and chemotherapy; Pt complexes as anticancer drugs; Complexes of gold as drugs.

Introduction to Bioinorganic chemistry of iron; metallo-porphyrins, heme protein- hemoglobin, myoglobin, cytochromes- structure and function, chlorophyll, photosynthesis: PS I and PS II

PAPER: CHEM 1002C

Organic Chemistry-IV

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I: Heterocyclic Chemistry (1 credit)

Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; Basicity and aromaticity of heterocycles; Synthesis, properties and reactions (ring openings & heteroatom extrusion) of 3- membered heterocycles (aziridines, oxiranes and thiiranes), 4- membered heterocycles (azetidine, oxetanes and thietanes); Synthesis and reactivity of azoles (imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiazole & their benzo derivatives) and azines (6- membered heterocycles with two hetero atoms -pyridazines, pyrimidines and pyrazines), caffeine; theobromine and theophylline.

Unit – II: Chemistry of natural products (0**1 credit):**

General classification of natural products; Isolation, characterization and biosynthetic studies of common natural products viz. terpenoids and steroids, phenolics, alkaloids; Chemistry of caryophyllin, isocaryophyllin, abeatic acid, cholesterol, estrogen and progesterone; Chemistry of quinine and morphine groups of alkaloids, lysergic acid and reserpine.

Suggested reading:

1. Heterocyclic Chemistry Vol. 1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T. L. Gilchrist, Pearson Education.
5. Contemporary Heterocyclic Chemistry, G. R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductiion to the Heterocyclic Compounds, R. M. Acheson, John-wiely.

7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.
8. Medicinal Natural Products, A Biosynthetic Approach 3rd Edition, Paul M Dewick, *John Wiley & Sons Ltd.*
9. Organic Chemistry Volume 2: Stereochemistry and the Chemistry of Natural Products, I. L. Finar, Fifth Edition, ELBS.
10. R.T. Morrison and R.N. boyd, Organic chemistry, 6th edn, Prentice hall of India, New delhi, 2003.

PAPER: CHEM 1003C

Physical Chemistry-IV

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT – I (Credit: 01)

A. ELECTROCHEMISTRY–I: Activity in electrolytic solutions. Freezing point depression and the mean ionic activity coefficient. The Debye-Huckel theory for dilute ionic solutions (derivation) and correction for concentrated solutions Equilibrium in ionic solutions. Ion association.

B. ELECTROCHEMISTRY–II: Electrodics - The basic electrodic equation: Butler-Volmer equation, over potential, polarisable and non-polarizable interfaces; Faradaic and non - faradaic Currents, Over-potentials, aspects of deviation from equilibrium. Electrical conductance of solutions; The Debye Huckel Onsagar equation for conductance (derivation); Conductance at high fields and high frequencies, Conductance in non-aqueous solvents. Fuel Cells: H_2-O_2 cell, Air-H cell; Electricity producing cells: Na-S, Sb-S.

Numerical problems.

UNIT-II (Credit: 01)

C. BIO-PHYSICAL CHEMISTRY: Hydrophobic effect and self organising systems, structure and functions of proteins and nucleic acids and their stability. Structure and functions of cell membranes; Ion transport through cell membranes and nerve conduction; Multiple equilibria; stacking and cooperative interactions in biological systems. Muscle contraction; Techniques for study of structure and functions of proteins and nucleic acids.

D. CHEMICAL KINETICS-II: Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple; Bi-molecular reactions; Collision theory; Activated complex theory. Reactions in solutions: Diffusion controlled and activation controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength; Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed uni-molecular and bimolecular reactions; Applications in ammonia synthesis and oxidation of carbon-monoxide.

Reference books:

1. J.O'M, Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Vol.1&2 (1998), Plenum Press, New York.
2. K. J. Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
3. H. Eyring, S. H. Lin and S. M. Lin, *Chemical Kinetics* (1999), Jhon Willey, New York.
4. K. Zeemanski, *Thermodynamics*

PAPER: CHEM 1004C

Supra-molecular and Nano Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit – 1 (Credit-01)

SUPRAMOLECULAR CHEMISTRY: Concepts and Languages of supramolecular chemistry - Molecules, super molecules and supramolecular Chemistry; factors leading to strong binding (non-covalent interactions); molecular receptors – design and principles; Types of interactions between host and guest molecules; Thermodynamics of host-guest complexation; Enthalpy and entropy contributions, complexation free energies; Molecular recognition – factors involved; Molecular receptors – for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, ionophores, cyclodextrins and calixaranes and their applications in specific recognition processes; Threading of a linear molecule through a cyclic molecule. Creation of rotaxanes and catenanes; Supramolecular catalysis- Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules; Catalysis with Cyclophane Type Receptors; Catalysis of Synthetic reactions; Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions; Applications - Supramolecular Devices and Sensors: Various types of supramolecular devices-Molecular and Supramolecular Photonic Devices – Light conversion and Energy transfer Devices. Molecular and Supramolecular Electronic Devices – Electronic conducting Devices - Molecular wires, Modified and Switchable Molecular wires. Molecular and Supramolecular Ionic Devices –Switching Devices: Photo switching and Electro switching. Role of supramolecular chemistry in the development of nanoscience and technology.

Unit -2 (Credit-01)

NANO CHEMISTRY: Background to Nano-science Science and Technology - Implications for Physics, Chemistry, Biology and Engineering - Classifications of nanostructured materials - nano particles - quantum dots, Nanowires, nano-tubes – ultra – thinfilms – multilayered materials. Typical syntheses of nano particles, oxide nano tubes and fibres, metal nano particles; Length Scales involved and effect on properties: Mechanical, Electronic, Optical, Magnetic and Thermal properties.

Synthesis of nanoparticle: Bottom-up Synthesis -Top-down Approach: Precipitation, Mechanical Milling, Colloidal routes, Self-assembly, Vapour phase deposition, MOCVD, Sputtering, Evaporation, Molecular Beam Epitaxy, Atomic Layer Epitaxy, MOMBE.

Characterization of nano particles- X-ray diffraction technique, Scanning Electron Microscopy - environmental techniques, Transmission Electron Microscopy including high-resolution imaging, Surface Analysis techniques

Application of nano-structured material in organic synthesis, dendrimers, bucky balls and nano tubes (properties and applications), drug delivery systems; Nanotechnology for sustainability, Nanomedicine, Environmental, health, and safety issues

Suggested reading:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. A.S. Edelstein and R.C. Cammearata, eds., Nanomaterials: Synthesis, Properties and Applications, (Institute of Physics Publishing, Bristol and Philadelphia, 1996)
3. N John Dinardo, Nanoscale charecterisation of surfaces & Interfaces, Second edition, Weinheim Cambridge, Wiley-VCH, 2000
4. G Timp (Editor), Nanotechnology, AIP press/Springer, 1999
5. Akhlesh Lakhtakia (Editor) The Hand Book of Nano Technology, "Nanometer Structure", Theory, Modeling and Simulations. Prentice-Hall of India (P) Ltd, New Delhi, 2007.

PAPER: CHEM 1005C

Chemistry Project - II

Total Marks: 100 (Project 70 + Internal Assessment 30)

Credits: 04

PAPER: CHEM 1007E

Bio-Inorganic Chemistry -II

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit 1 Metallo proteins and metalloenzymes: Fe, Cu, Zn, Mn,- Hemerythrin, ferritin, transferrin, bio-mineralization and siderophores, peroxidase, catalase, cytochrome P-450, iron-sulphur proteins, rubredoxins, ferredoxins, blue-copper proteins, ceruloplasmin, hemocyanin, cytochrome C oxidase, superoxide dismutase, carbonicanhydrase, Alcohol dehydrogenase, Carboxypeptidase, metallothionein, inter changeability of Zn and Co in enzymes.

Unit II Biochemical role of Co Mo and W- Biological nitrogen fixation, vitamin B_{12}, B_{12} coenzyme, cobalamin, nitrogenase, Xanthine oxidase, sulphite oxidase, nitrite reductase, Arginase, Mn-SOD, chlorophyll, Photosystem I and II, cleavage of water.

Unit III Metals in medicine: Toxicity of Hg, Cd, Pb, Cr, Be, Se, and As. Biological defence mechanism, Chelation therapy, metals used for diagnosis and Chemotherapy, Pt-complexes as anticancer drugs, Complexes of gold, copper, Zn, Hg, As as drugs.

PAPER: CHEM 1008E

Environmental and Green Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit – I: Environmental Chemistry (Credit – 01)

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, Ozone depletion, The green-house effect and Global warming, El-Nino phenomenon. Micro-organism in aquatic chemical reactions, Eutrophication, Re-cycle of waste-water in process industry, Treatment of sewage and reuse of water in industry and agriculture, microbiologically mediated redox reactions and Nitrogen transformation by bacteria. Water pollutants: Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity, DO, BOD, COD etc.); industrial and waste-water treatment; Chemical hazards, chemical disaters, pollution of environment-man made, industrial, natural disasters, environmental biochemistry, toxicological chemistry; analysis of water and waste water, solid wastes and air pollution-Photochemical smog, Auto exhausts, Acid-rains, Air-quality standards. Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

Unit – II: Green Chemistry (Credit – 01)

Definition, Concepts and basic principles of green chemistry, need of green chemistry, green chemistry as an alternative tool for reducing pollution, atom economy, less hazardous chemical syntheses, atom economy in rearrangements, addition and pericyclic reactions, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, Green synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology. Development of new methods for organic synthesis such as Green Synthesis: use of sonochemistry, use of ionic liquids, use of microwaves, bio-catalysis. Selection of solvent: i) Aqueous phase reactions ii) Reactions in ionic liquids iii) Solid supported synthesis iv) Solvent free reactions, Green catalysts: i) Phase transfer catalysts (PTC) and ii) Biocatalysts. Microwave and Ultrasound assisted green synthesis: Aldol condensation, Cannizzaro reaction, Diels-Alder reactions, Strecker synthesis, Willaimson synthesis and Dieckmann condensation.

Book Suggested:

1. *Handbook of Environmental chemistry*, Springer-Verlag, O. Hutzinger.
2. M. Bernhard, F.E. Brinckman & P.J. Sadler.*The Importance of Chemical Speciation in Environmental Processes*, Springer-Verlag,
3. L.J. Fristschen, & L.W. Gay, *Environmental Instrumentation*, Springer-Verlag,.
4. Real World Cases in *Green Chemistry*, ACS, M.C. Cann & M.E. Connelly.
5. P.T. Enastas and T.C. Williamson, Green Chemistry: Designing Chemistry for Environment, ACS,
6. *Green separation processes, methods and application*, Fonso, National Scientific Book Agency, Delhi-110053.
7. G.W. Vanloon, S.J. Duffer, *Environmental Chemistry* - A Global Perspective, (2000) Oxford University Press.
8. F.W. Fifield and W.P.J. Hairens, *Environmental Analytical Chemistry*, 2nd Edition (2000), Black Well Science Ltd.
9. Colin Baird, *Environmental Chemistry*, (1995) W.H. Freeman and Company, New York.
10. A.K. De, *Environmental Chemistry*, 4th Edition (2000), New Age International Private Ltd., New Delhi.
11. Peter O. Warner, *Analysis of Air Pollutants*, 1st Edition (1996), John Wiley, New York.
12. S.M. Khopkar, *Environmental Pollution Analysis*, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
13. S.K. Banerji, *Environmental Chemistry*, 1st Edition (1993), Prentice-Hall of India, New

PAPER: CHEM 1009E

Advanced Spectroscopic techniques

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I: C-13 NMR Spectroscopy:

Chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon);

Coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies.

Unit II: ***Applications*** of IR, NMR and Mass spectroscopy for structure elucidation of organic compounds.

PAPER: CHEM 1010E

Chemistry of Natural products

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT – I

General: Sources and types of natural products, method of isolation and structure elucidation, importance of natural products, biosynthesis of some common type of natural products – terpeneoids, steroids, flavonoids and alkaloids.

Chemistry of terpenoids, **steroid and hormones:** Terpenoids – sesquiterpenoids, diterpenoids with special reference to the isolation, structure and stereochemistry: alpha-santonin, Caryophyllene and isocaryophyllene, abietic acid and Gibberellic acid.

Steroids and hormones – Cholesterol, oestrone, progesterone, testosterone.

UNIT- II Alkaloids and Phenolics - Chemistry of quinoline, isoquinoline, phenanthrene and indole group of alkaloids - papaverine, cimchonine quinine, morphine, thebaine, codeine, reserpine with special reference to isolation, structure and stereochemistry. Plant phenolics with special reference to the general structures, reactions and synthesis of anthocyanins, anthocyanidins, flavones flavonols, isoflavones, chalcones, coumarins, quinines and tannins.

Reference books:

1. Organic Chemistry, I.L. Finar, volume 2, ELBS, 5th edition (1975).
2. Organic Chemistry. Morrison Boyd and Bhattacharjee, 7th edition (2013), Pearson.

PAPER: CHEM 1011E

Medicinal Chemistry-II

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit 1 ***Drug Types - I***

*(a) Antineoplastic drugs***:** Cancer chemotherapy, role of alkylating agents and antimetabolites in the treatment of cancer; Carcinolytic antibiotics and mitotic inhibitors; Synthesis of mechlorethamine, melphalan, 5-bromouracil and 6-mercaptopurine; Anticancer action of cisplatin and taxol.

*(b) Cardiovascular drug***:** Classification, synthesis and mode of action of quinidine, verapamil, methyldopa and buphenine.

*(c) Hypnotics and sedatives***:** SAR and mode of action; Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, barbiturates, thiopental sodium.

*(d) Local anaesthetics***:** Classification, SAR and mode of action; Synthesis of procaine, α-eucaine and β-eucaine, xylocaine, cinchocaine and quinisocaine.

Unit 2 ***Drug Types - II***

*(a) Antiinfective drugs***:** Mode of action and synthesis of sulphonamides, furazolidone, ciprofloxacin, norfloxacin, daspone, isoniazide.

*(b) Antipyretic Analgesics***:** Classification and mode of action of antipyretic analgesics; Synthesis of paracetamol, chincophan, Novalgin and mefenamic acid.

*(c) Antihistamines***:** SAR and mode of action of H1-receptor antagonists; Synthesis of bromazine, mepyramine, methapyriline, antazoline, promethazine and phenindamine.

*(d) Antimalarial drug***:** Nitrogen heterocycles as antimalarial agents, their classification and mode of action, synthesis of chloroquine, pamaquine, primaquine, Mepacrine and pyrimethamine. Introductory idea on Artemisinin, artemether and arteether.

PAPER: CHEM 1012E

Photochemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT- I (Credit- 01):

Physical properties of excited molecules: Nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids. Polarised luminencence, non radiative intra-molecular electronic transition, internal conversion, intersystem crossing, crossing potential energy surface (Franck- Condon factor).

UNIT- II (Credit – 02)

Photo-physical processes in excited state: Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation. Mechanism of quenching, energy transfer process (Forster dipole coupling), electron transfer phenomenon (Marcus theorem, Rehm Weller theorem), eximer.

Applications of photochemistry: Importance of photochemistry, origin of life, photosynthesis and mechanism of vision.

Reference books:

1. K. K. Rohtagi-Mukherjee, *Fundamental of Photochemistry*,(1986) New Age International New Delhi.
2. J. G. Calvert and J. N. Pitts, Jr., *Photochemistry* (1966) John Wiley & Sons, New York.
3. R. P. Wayne, *Principles and Application of Photochemistry* (1988), Oxford University Press, Oxford.
4. N. J. Turro, *Modern Molecular Photochemistry*, (1991) Univ. Science Books, Sansalito.
5. J. F. L Lakowicz, *Principles of Fluorescence Spectroscopy*, 2nd Edn. (1999) Planum Publishers, New York.

PAPER: CHEM 1013E

Fortran and C, C+, C++ Programming

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

FORTAN programming F77:

FORTAN programming preliminaries; FORTAN constants and variables; Arithmetic Expressions. Input-output statements. Simple computer programmes. Control statements. The Do statements. Subscripted variables. Elementary Format Specifications. Logical Expression. Function and subroutines. Processing files in FORTRAN. Use of common statements. FORTAN 90, 95(Introduction).

UNIT-II

C, C+ , C++

PAPER: CHEM 1014E

Statistical Mechanics

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

Classical monatomic liquids-radial distribution function (RDF); Relating RDF with the thermodynamic properties; integral equations; Potential of mean force; the direct correlation function.

Statistical mechanical perturbation theory of liquids: theory and its application to derive van der Waals equation of state.

UNIT-II: Non-equilibrium statistical mechanics: Random Processes; Time-correlation functions;

Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.

Reference books:

1. B. J. Mcclelland, *Statistical Thermodynamics*
2. M. Dole, *Introduction to Statistical Thermodynamics*
3. M. C. Gupta, *The statistical Thermodynamics* (1990), New Age International (P) Ltd. New Delhi
4. Anrew Maczek, S*tatistical Thermodynamics* (1978), Oxford University Press Inc. New York
5. D. A. McQuarrie, *Statistical Mechanics* (2003), Viva Books Pvt. Ltd. New Delhi.

Suryamaninagar 799022
West Tripura
India

NOTIFICATION

Date: 12.07.2017

This is for the information to all concerned that ,fourth (4th) meeting of Board of Post Graduate Studies (BPGS) of the Department of Chemistry (formed, Vide notification No.F.TU/DIR.CDC/BOF(Sc.)/80/2016 dt. 21.04.2016) shall be held on 28.07.2017 (Friday) at 12.30 p.m. in the Department of Chemistry, Tripura University to consider the following agenda. All the members are requested to attend the meeting.

Agenda:

1. Approval of Revised Course Structure for M.Sc,Chemistry.
2. Approval of class routine/ Academic calendar for 1st and 3rd semesters.
3. Approval of the revised M.Sc. syllabus 1st to 4th semesters.
4. Approval of Research Advisory Committee (RAC) for
   (i) Smt. Maitri Bhattacharjee
   (ii) Smt. Tania Modal
   (iii) Smt. Bijayashree Misra
5. Reports on Ph.D. Viva-Voce examination of Mr. Jewel Hossain
6. Holding of National Seminar.
7. Misc.

Prof. R.N. DuttaPurkayastha 11.7.17
Convener, BPGS (Chemistry)
Tripura University

Convener
Board of Post-Graduate Studies
Department of Chemistry
Tripura University
Suryamaninagar-799022

To:

1. Dean of Faculty of Science, T.U.
2. Head of the Dept. of Chemistry, T.U.
3. Prof. M.K. Singh, Dept. of Chemistry, T.U.
4. Prof. D. Sinha, Dept. of Chemistry, T.U.
5. Prof. R.K. Nath, Dept. of Chemistry, T.U.
6. Dr. S. Majumdar, Associate Prof., Dept. of Chemistry, T.U.
7. Dr. U.C. De, Asstt. Prof., Dept. of Chemistry, T.U.
8. Dr. S. Chowdhury, Asstt. Prof. Dept. of Chemistry, T.U.
9. Prof. S.K. Sil, Dept. of Human Physiology, T.U.
10. Prof. S.C. Bhattacharya, Dept. of Chemistry, Jadavpur University, Kolkata.
11. Prof. C.R. Bhattacharjee, Dept. of Chemistry, Assam University, Silchar.
12. Dr. Soumen Maiti, Senior Principal Research Scientist, TCG Life Sciences Limited, Kolkata.

Copy to:

1. P.S. to Hon'ble Vice-Chancellor, T.U. for kind information
2. Controller of Examinations, T.U.

Proceedings of the 41st BPGS meeting of the Department of Chemistry, held on 28.07.2017 at 12.30 P.m.

Members present

1. Prof. M. K. Singh —
2. Prof B. Sinha 28.7.17
3. Prof R. K. Nath
4. Prof. S. Majumdar — 28/7/17
5. Dr. U. C. De 28/7/17
6. Prof S. K. Sil —
7. Prof. S. C. Bhattacharyee (External member) Bhattacharyee 28.7.17.
8. Prof. R. N. Dutta Purkayastha (Convenor) 28/7/17

DEPARTMENT OF CHEMISTRY
TRIPURA UNIVERSITY
(A Central University)
Suryamaninagar 799022
West Tripura
India

Phone: +91-381 2379071
Fax: +91-381 234802

Proceedings of the 4th meeting of Board of Post Graduate Studies in Chemistry of Tripura University held on 28.07.2017 at 12.30 p.m. in the Department of chemistry.

Members Present:

1.	Prof. D. Sinha	Member, Dept. of Chemistry, TU
2.	Prof. R.K. Nath	Member, Dept. of Chemistry, TU
3.	Prof. S. Majumdar	Member, Dept. of Chemistry, TU
4.	Dr. U.C. De	Member, Dept. of Chemistry, TU
5.	Prof. R.N. Dutta Purkayastha	(Convener), Dept. of Chemistry, TU
6.	Prof. S.C. Bhattacharya	Department of Chemistry, Jadavpur University(external Member)

At the outset Convener extended a warm welcome to the members present in the meeting.

After a brief introduction by the Convener, proceeding of the 3rd meeting of BPGS held on 21.03.2017 was read out and confirmed with some modifications. Thereafter, the agenda items were discussed as per the notification of the meeting. The following resolutions adopted in the meeting after thorough discussion.

Agenda 1 Approval of Revised course structure for M.Sc. Chemistry.

Resolution The revised course structure for the M.Sc. 1st to 4th semesters was discussed in details by the member and approved for implementation from the academic session July- Dec '2017 (copy enclosed)

Agenda 2 Approval of class routine / Academic calendar for 1st and 3rd semester.

Resolution The provisional class routine and Academic calendar for the Academic session July-Dec'2017 was discussed and approved.

Agenda 3 Approval of revised M.Sc. syllabus 1st to 4th semester.

Resolution: Contents of the proposed revised syllabus was considered thoroughly, After detailed discussions and incorporating valuable suggestion from the members , the proposed revised syllabus was approved for implementation from the Academic session July-Dec'2017.

Agenda 4 Approval on the Research Advisory Committee (RAC) for (I) Smt. Matri Bhattacharjee , (II) Smt. Tania Mondol (III) Smt. Bijayashre Mishra

Resolution: The proposed names of Research advisory committee (RAC) members for the candidates Smt. Matri Bhattacharjee , Smt. Tania Mondol , Smt. Bijayashre Mishra as proposed by the respective supervisors were approved The composition of the committees are as follows.

(a) Candidate, Smt. Matri Bhattacharjee
RAC members
(1) Prof. R.N. Dutta Purkayastha Dept. of Chemistry, TU (Convener Supervisor)

DEPARTMENT OF CHEMISTRY

TRIPURA UNIVERSITY

SURYAMANINAGAR – 799022

M. Sc. CHEMISTRY SYLLABUS

CHOICE-BASED CREDIT SYSTEM

(Revised 2017)

DEPARTMENT OF CHEMISTRY
TRIPURA UNIVERSITY
SURYAMANINAGAR 799 022
CHOICE BASED CREDIT SYSTEM (REVISED 2017)*

Course Curriculum – M. Sc. in Chemistry, Tripura University

Course Code	Name of the Courses	Credits
Semester –I (12 Credits core)		
CHEM 701C	Inorganic Chemistry-I	02
CHEM 702C	Organic Chemistry-I	02
CHEM 703C	Physical Chemistry-I	04
CHEM 704C	Chemistry Practical-I	04
Elective (Compulsory)		
CHEM 704E	Statistics	04
CHEM 705E	Computer	04
Semester – II (12 Credits core)		
CHEM 801C	Inorganic Chemistry-II	02
CHEM 802C	Organic Chemistry-II	04
CHEM 803C	Physical Chemistry-II	02
CHEM 804C	Chemistry Practical-II	04
Elective		
CHEM 805E	Spectroscopic Techniques in inorganic Chemistry	02
CHEM 806E	X-ray Crystallography and Solid state chemistry	02
CHEM 807E	Chemistry of Bio Molecules-I	02
CHEM 808E	Medicinal Chemistry	02
CHEM 809E	Advanced Group Theory	02
CHEM 810E	Surface Chemistry	02
Semester – III (12 credits core)		
CHEM 901C	Inorganic Chemistry-III	04
CHEM 902C	Organic Chemistry-III	02
CHEM 903C	Physical Chemistry-III	02
CHEM 904C	Chemistry Project-I	04
Elective		
CHEM 905E	Analytical and separation techniques in chemistry	02
CHEM 906E	Enzyme Chemistry	02
CHEM 907E	Bio-inorganic chemistry	02
CHEM 908E	Chemistry of Bio Molecules-II	02
CHEM 909E	Polymer Chemistry	02
CHEM 910E	Quantum Mechanics – II	02
Semester – IV (12 Credits core)		
CHEM 1001C	Inorganic Chemistry-IV	04
CHEM 1002C	Organic Chemistry-IV	02
CHEM 1003C	Physical Chemistry-IV	02
CHEM 1004C	Chemistry Project-II	04
Elective		
CHEM 1005E	Supra-molecular and Nano Chemistry	02
CHEM 1006E	Environmental and Green Chemistry	02
CHEM 1007E	Chemistry of Natural Products	02
CHEM 1008E	Photochemistry	02
CHEM 1009E	Computer Programming	02
CHEM 1010E	Statistical Mechanics	02

*Total minimum 72 credits should be obtained; core courses and two electives in first semester are compulsory

Convener 12/07/2017
Board of Post Graduate Studies
Department of Chemistry
Tripura University
Suryamaninagar-799022

First Semester courses from the Department of Chemistry

Course Code		Name of the Courses	Credits
CHEM	701C	Inorganic Chemistry-I	02
CHEM	702C	Organic Chemistry-I	02
CHEM	703C	Physical Chemistry-I	04
CHEM	704C	Chemistry Practical-I	04

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INORGANIC CHEMISTRY - I
PAPER – CHEM 701C

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit-I Symmetry and Group Theory:

(a) Symmetry elements and operations, equivalent symmetry elements and equivalent atoms, point groups with examples, Group of very high symmetry, systematic procedures for symmetry classification of molecules and illustrative examples, molecular symmetry for compounds having coordination number 2 to 9, molecular dissymmetry and optical activity.

(b) Elementary idea of representation of theory, brief review of matrix, representation of groups, reducible and irreducible representation of point groups, definition of classes and character, the "Great Orthogonality Theorem", Orthogonality theorem for character tables, concept of character projection operator. Utilization of symmetry and group theory in constructing MO diagrams for polyatomic molecules (AB_n), the normal mode of vibration, symmetry of normal vibration, selection rules for IR and Raman Transitions.

Unit-II Stereochemistry and Bonding:

(a) VSEPR Theory; VBT (diatomic molecule); Polyatomic molecules; hyper-valence; localized bond, hybridization and energetics of hybridization; dπ-pπ bond; Bent's rule; Walsh Diagrams; MOT (simple LCAO); σ, π, δ M.O.; bonding and antibonding M.O. orbitals; criteria for stable molecular orbitals; orbital symmetry and overlap; homo-nuclear diatomic molecules; hetero-nuclear diatomic molecule; polyatomic molecules; molecular shapes in terms of molecular orbitals.

(b) Structure and bond properties; bond length, bond strength, electronegativity, group electronegativity, bond enthalpy, bond polarity, weak interactions:- hydrogen bonding, metallic bonding – band Theory, bonding in alloys, intermetallic compounds.

Text Books and suggested readings:

1. J. E. Huheey, E. A. Keiter, R. L Keiter and O. K. Medhi. Principles of Structure and Reactivity. First impression, Pearson Education 2006.
2. F. A. Cotton. Chemical Applications of Group Theory (3rd Edn) John-Wiley and Sons.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry (5th edition) John Wiley
4. R. L. Dutta and A. Syamal, Elements of Magnetochemistry.
5. W. L. Jolly, Modern Inorganic Chemistry.
6. Gary L. Miessler and Donald A. Tarr, Inorganic Chemistry (4th Edition)
7. David M. Bishop Group Theory and Chemistry (Dover Books on Chemistry)
8. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, Shriver and Atkins Inorganic Chemistry, Oxford University Press (2006).
9. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984).
10. S. F. A. Kettle, Physical Inorganic Chemistry, Spectrum (1996).

ORGANIC CHEMISTRY -I

PAPER: CHEM 702C

Total Marks: 50 (Theory 35+ Internal Assessment 15)

Credit: 02

Unit I: Organic reaction mechanism

HSAB principle and its application in organic chemistry; Kinetic and non-kinetic methods for determination of reaction mechanisms; Linear free energy relationship; the Hammett equation-substitution and reaction constants; addition reactions of allenes and carbonyl compounds, stereochemistry of substitution, addition and elimination reactions; Substitution vs elimination reactions; neighboring group participation and anchimeric assistance.

Aromaticity; mechanism of formation of different aromatic ions and their stability

Unit II: Orbital symmetry reaction

Introduction to pericyclic reactions, orbital symmetry, electrocyclic, cycloaddition, sigmatropic and group transfer reactions; Woodward-Hoffmann rule and orbital motions in different pericyclic reactions; Rationalization based on FMO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Chelatropic reactions, Cope, aza-Cope, oxy-Cope, Claisen, Somelett-Hauser rearrangements.

Unit III: Reactive intermediates –I:

Introduction-structure, reactivity and stability of carbocations, carbanions, carbenes and nitrenes; Reactions involving these intermediates: pinacol-pinacolone rearrangement, Demjenov rearrangement, dienone-phenol rearrangement, Wolf rearrangement, cyclopropanation, Simon-Smith reaction, rearrangement of acylnitrenes etc.

Recommended text and reference books:

1. F. A. Carey and R. J. Sundberg. Advanced Organic Chemistry. 5thEdn. Plenum. Part – I, Part – II.
2. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4thedn, John Willey
3. R.T. Morrison and R.N. Boyd, Organic chemistry, 6thedn, Prentice hall of India, New Delhi, 2003.
4. Michael B. Smith & Jerry March, Advanced Organic Chemistry Reactions, Mechanisms, and Structure. (2013) Wiley-Interscience.
5. T. Laue and A. Plagens, Named OrganicReactions,2nd edition (2005), John Wiley & Sons Ltd.
6. Reinhard Bruckner Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
7. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press.
8. A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.
9. B. Dinda, Essential of Pericyclic and organic photochemistry, Springer (2016).
10. J. Sing & J Singh, Photochemistry and pericyclic reactions, New Age International (Pvt. Ltd). 3rd Edition (2010).
11. Paula Y. Bruice, Organic Chemistry, Pearson, Seventh Edition (2016).
12. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, John Wiley & Sons Inc. 5th Edition.
13. Herbert O. House, Modern Synthetic Reactions, 2nd edition, The Benjamin/Cumings Publihing Company.

PHYSICAL CHEMISTRY - I

PAPER: CHEM 703C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

Group A: Marks- 50

UNIT –I

QUANTUM MECHANICS-I:

General Principles of Quantum Mechanics

Introduction; linear operators; Hermitian operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; separability of Schrodinger equation ; equation of motion.

Application to Simple Systems and Approximation Methods

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential, tunnelling effect and hydrogen atom. Antisymmetry principle and many-electron wave finctions.

Chemical Bonding

Born-Oppenheimer approximation (Introduction); valence bond (VB) theory and molecular orbital (MO) theory for diatomic molecules – hydrogen molecule ion, hydrogen molecule; excited states of H_2 – singlet and triplet; non-crossing rule and correlation diagram.

UNIT-II: SPECTROSCOPY-I

Rotational (microwave) spectra, rigid diatomic molecule, Energy expression; Rotational constant. Selection rules. Determination of bond length from observed rotational spectra. Spectral intensity-degeneracy of rotational energy levels and total relative population. The effect of isotopic substitution. Non-rigid rotator (energy expression only).Chemical analysis by microwave spectroscopy.

Vibrational (infra-red) spectra:Simple harmonic oscillator model. Corresponding selection rule. Anharmonic oscillator model-Morse function. Selection rules. Fundamental absorption and overtones. Hot bands. P-,Q-,R- branch in IR spectra. IR spectra of linear molecules. Parallel and perpendicular vibrations. Chemical analysis by IR techniques.

Raman spectroscopy: Rayleigh scattering and Raman scattering (classical and quantum mechanical consideration). Stokes and Anti-stokes lines. Selection rule. O- and S-branch in Raman spectra. Rotational Raman spectra of homonuclear diatomic molecules. Vibrational Raman Spectra .The rule of mutual exclusion. Structure determination from Raman and IR spectra.

Numerical problems.

Group B: Marks- 50

UNIT-III: Spectroscopy -II

NMR spectroscopy: Theory for NMR Population of energy levels. Larmor precession. Relaxation times: spin - lattice relaxation, spin-spin relaxation. Fourier transform spectroscopy in NMR . Chemical shift. Shielding and de-slielding mechanism. Fine structure, spin-spin splitting, coupling constant. Strongly coupled systems, shift reagent in NMR. Hyperfine structure. Nuclear overhauser effect (NOE), 1H and ^{13}C NMR. Two-Dimentional NMR. Chemical analysis by NMR techniques.

ESR spectroscopy : General background of ESR spectroscopy .Representation of ESR spectrum. 'g' - value, ESR spectra of simple organic free radicals; Hyperfine coupling, prediction of expected number of lines and their relative intensities, ESR spectra of transition metal complexes, metal-hyperfine coupling, anisotropic ESR spectra, zero field splitting, application of ESR spectroscopy examples.

UNIT-IV: Spectroscopy -III

***Photoelectron Spectroscopy (PES)*:** Frank- Condon principle, Basic principles of photoelectron and X-ray photoelectron spectroscopies and their applications for chemical analysis of surfaces; application of ESCA and Auger spectroscopy for the studies of solids.

NQR: Nuclear quadruple resonance, Energy levels of a nucleus in a non-uniform electric field. Quadruple coupling constant. NQR spectra of molecular compounds.

Mossbauer Spectroscopy: Principles of Mossbauer spectroscopy, Doppler shift, Application of Mossbauer spectra for chemical structure determination, Numerical problems.

Reference books:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. D. A. MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
3. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, Tata McGraw Hill, 1997.
4. I. Levine, *Quantum Chemistry*, (1994)Tata McGraw Hill, New Delhi.
5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, (1935), McGraw Hill, New York.
6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
7. Molecular Spectroscopy by G. Aruldhas
8. Molecular Spectroscopy by G. M. Barone
9. Molecular Spectroscopy by Banwell
10. Molecular Spectroscopy by Ira N Levine.

CHEMISTRY PRACTICAL-I

Paper: CHEM 704C

Credit: 04

Group A: Laboratory Course in Inorganic Chemistry

1. Semi micro qualitative analysis of Inorganic salt mixtures containing (06) six radicals including W, Mo, V, Ti, U, Th, Zr, Ce and at least one interfering radical (F^-/PO_4^{3-}/BO_3^{3-}).
2. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three component mixtures and alloys.
3. Preparation of the following inorganic compounds and characterization by IR, UV-Vis, Conductance & magnetic susceptibility measurements.
   Tris (acetyl acetonato)manganese (III)
   Tris (acetyl acetonato)iron (III)
   Linkage isomer of nitro & nitrido pentammine Cobalt (III) Chloride
   Tris (Ethylene diammine) Nickel (II) Chloride. dehydrate

Group B: **Laboratory Course in Physical Chemistry**

1. Determination of specific rotation of cane sugar and determination of concentration of supplied sample.(Quantitative-one day).
2. Potentiometric titration of Co(II) by $K_3[Fe(CN)_6]$ and determination of concentration of Co(II) in a solution. (Quantitative-one day).
3. Conductomectric titration of triple mixture containing KCl, NH_4Cl and HCl by $AgNO_3$ and by NaOH solution. (Quantitative-one day).
4. Verification of Beer's law and determination of concentration of unknown solution spectrophotmetrically(Quantitative-one day).
5. Determination of strengths of halides in a mixure , potentiometrically.
6. Determination of pH of buffer solutions and hence to calculate the E0 of quinhydrone electrode
7. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
8. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.

Semester – II (12 Credits core)

CHEM	801C	Inorganic Chemistry-II	02
CHEM	802C	Organic Chemistry-II	04
CHEM	803C	Physical Chemistry-II	02
CHEM	804C	Chemistry Practical-II	04

Elective

CHEM	805E	Spectroscopic Techniques in inorganic Chemistry	02
CHEM	806E	X-ray Crystallography and Solid state chemistry	02
CHEM	807E	Chemistry of Bio Molecules-I	02
CHEM	808E	Medicinal Chemistry	02
CHEM	809E	Advanced Group Theory	02
CHEM	810E	Surface Chemistry	02

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INORGANIC CHEMISTRY - II
PAPER – CHEM 801C
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit-I Coordination Chemistry

Brief review of theories of coordination compounds (VBT, CFT), Ligand Field Theory (LFT), Experimental evidences for metal-ligand orbital overlap, Calculation of ligand field parameters for complexes, MO Theory (LCAO) for complexes, application of MOT to octahedral, tetrahedral and square planar complexes, π-bonding in octahedral complexes and its effect on energy of molecular orbitals.

Unit-II Magneto-chemistry

Different types of magnetic behaviour of materials and their origin, magnetic susceptibility and magnetic moment, measurement of magnetic susceptibility (Gouy and Faraday methods), quenching of orbital moments, Interpretation of magnetic moments of complexes on the basis of various theories of complexes.

Magnetic behavior of multi-electron system, orbital coupling, spin-coupling, spin-orbit coupling (Russel Saunder's coupling), spin-orbit coupling constant, spin-orbit interaction energy, j-j coupling, micro-states and term symbols, Hund's rule for ground state term symbol, Lande interval rule, Derivation of Curie equation for magnetic moment, Curie and Curie-Weiss law, Thermal energy and magnetic moment, anti-ferromagnetism and its exchanged pathways.

Unit – III Bioinorganic Chemistry -1

Essential and trace element in biological system. Structure and function of biological membranes, mechanism of ion transport across membranes; Crown either complexes of Na and K, Ionophores, Valinomycin, Sodium and Potassium pump; Catalysis of phosphate transfer by Mg^{2+} ion; Metalloporphyrins: Structure and function.

Suggested reading:

1. Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn. J. Huhee, E.A. Keiter, R.L.Keiter & O.K. Medhi Pearson Education, New Delhi.
2. Shriver & Atkins - Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
3. Bioinorganic Chemistry, Asim K. Das, Books & Allied Ltd, 2013.
4. Bioinorganic Chemistry (Bertini, Ivano; Gray, Harry B.; Lippard, Stephen J.; Valentine, Joan Selverstone), University Science Books, CA, 1994.

ORGANIC CHEMISTRY - II
PAPER – CHEM 802C

Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 02

Group A

Unit I: Advanced Stereochemistry

Symmetry elements and point groups, axial and planar chirality, correlation of axial dissymmetry and Centro dissymmetry, atropisomerism, stereochemistry of allenes, biphenyls and spiro compounds. Topicity, acyclic systems up to 4 chiral centers, Compounds with asymmetric carbons in branched chains, asymmetric synthesis, Winstein- Holness equation and the Curtin- Hammett principle, conformational analysis of cyclic compounds such as substituted cyclohexanes, fused ring systems (decalins, PHA, PHP), allylic strains, alkylketone effects, haloketone rule.

Unit –II: Reactive intermediates - II

Arynes: Generation, structure and stability; Benzyne mechanism for aromatic nucleophilic substitution; Rearrangement and cyclo-addition reactions of arynes, synthetic application.
Enamines: Generation, structure and stability of enamines; synthetic applications.
Free radicals: Generation, structure and stability of radicals, radical- initiator, scavenger substitution and addition reactions involving radicals,tributyl tin hydride mediated radical reactions, exo- and endo cyclisation.

Group B

Unit I: Strategies and reagents in organic synthesis

Designing of organic synthesis - Retrosynthetic and Disconnection approach; Reversal of dipoles (umpolung of reactivity) and it's applications; Synthons and retrons, linear and convergent synthesis, protection and deprotection strategies, protecting agents for common functional groups; Trans metallation approach and metal catalyzed cross coupling reactions.

Uses of the following reagents/reactions in organic synthesis: PCC, PDC and Collin's reagent; IBX, Dess-Martin periodinane, ceric ammonium nitrate, Thallium(III) nitrate, chloranil, DDQ, m-CPBA, K-selecteride and L-selecteride, sodium cyanoborohydride, super hydrides, 9-BBN, Mukaiyama reagent, Gilman's reagent, LDA, dicyclohexylcarbodimide, tri-n-butyltin hydride, NCS, NBS, NIS, Corey-Nicolaou reagent, baker's yeast, CBS reagents, diimide, crown ether, phase transfer catalyst.

Unit III: Selective named reactions (1 credit)

Arndt Eistert synthesis, Swern oxidation, Moffat oxidation, Prevost and Woodward hydroxylation; Henry reaction, Wittig reaction and Horner-Wordwoth-Emmons reaction (stabilized and non-stabilized ylide); Nazarov cyclization, Pictet-Sprengler reaction, Biginelli reaction, Passerini reaction, Ugi reaction, Peterson's synthesis, McMurry olefination, Julia olefination, Tebbe Olefination. Shapiro reaction, Chichibabin reaction, Baeyer-Villiger oxidation, Baylis-Hillman Reaction, Staudinger Reaction, Stobbe Condensation.

Recommended text and reference books:

1. W. Carruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University Press (2004).
2. L. Stryer, Biochemistry, 5th Edition (2002), Freeman & Co, New York.
3. H. O. House, Modern Synthetic Reactions, 3rd Edition (1992), Benjamin Publishing Co.
4. S. Warren, Organic Synthesis, Disconnection Approach, 1982, Wiley Interscience, NY
5. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry Part A and Part B.
6. T. Laue and A. Plagens, Named Organic Reactions,2nd edition (2005),John Wiley & Sons Ltd

7. *Reinhard Bruckner* Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
8. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press
9. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4thedn, J. Willey
10. D. Nasipuri, Stereochemistry, Conformation and mechanism, 2ndEdn. John Wiley
11. R.T. Morrison and R.N. Boyd, Organic chemistry, 6thedn, Prentice hall of India, New
12. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 2007.
13. S. Sengupta Basic Stereochemistry of Organic Moleclules, Book Syndicate Pvt. Ltd. 2nd Edition.
14. P.S. Kalsi, Stereochemistry, Conformation and Mechanism, 8th Edition. New Age Int., 2015.

PHYSICAL CHEMISTRY - II
PAPER – CHEM 803C
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

UNIT-I: CHEMICAL THERMODYNAMICS

Nernst heat theorem and the third law of thermodynamics, Calculation of entropy changes in chemical reactions, Mathematical and thermodynamic probability. Entropy and probability. The free energy of a mixture. Dependence of thermodynamic functions on composition. Partial molar quantities.

Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures. Concept of fugacity.

Analytical form of the chemical potential in ideal solutions. Chemical potential of the solute in a binary solution Application of Gibbs-Duhem equation.

The concept of activity:the rational concept and the practical concept. Colligative properties and activity of solute. Activities and reaction equilibria, experimental determination of activity coefficients of non-electrolytes, Numerical problems.

Unit -II: Kinetic theory and transport properties of gases

Derivation of Maxwell's distribution of molecular speed**;** The general equation for transport, Thermal conductivity of gases, Molecular collisions and mean free path, Viscosity of gases, Diffusion , Introduction to the concept of non-steady state, Numerical problems.

Unit-III: Chemical kinetics-1

Opposing and consecutive reactions, complex reactions, Atomic and free radical chain reactions. Kinetic salt effect; Effect of solvent on rate constant (Single sphere and double sphere model): Non-Arrhenius equations and its significance. Theory of absolute reaction, rate (statistical) and comparison with that of collision theory; Kinetics of enzyme reaction (effect of pH) Michaels- Menton Law, derivation; Numerical problems

Reference books:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. D. A. MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
3. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, Tata McGraw Hill, 1997.
4. I. Levine, *Quantum Chemistry*, (1994)Tata McGraw Hill, New Delhi.
5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, (1935), McGraw Hill, New York.
6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
7. K.J.Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
8. H.Eyring, S.H. Lin and S.M.Lin, *Chemical Kinetics*, (1999)Jhon Willey, New York.
9. K. Zeemanski, *Thermodynamics*

CHEMISTRY PRACTICAL-II

PAPER: CHEM 804C

Credit: 04

Group A: Laboratory Course in Organic Chemistry

1. Separation, purification and identification of compounds of binary solid mixtures by systematic analysis
2. Identification of organic liquid compounds by systematic analysis
3. Organic preparation
4. Organic estimation - Estimation of some organic compounds

Group B: Laboratory Course in Physical Chemistry

1. Determination of rate constant and order of the reaction between $KBrO_3$ and KI in acid medium.(Qualitative- one day)
2. Kinetic study of decomposition of $K_2S_2O_8$ by KI and effect of added salt. (Qualitative- two day)
3. Determination of formula of cupro-ammonium ion. (Qualitative- one day)
4. Determination of distribution coefficient of C_6H_5COOH between H_2O and an organic solvent (verification of dimerization of benzoic acid in organic solvent). Qualitative- one day)
5. Determination of standard electrode potential of quinhydrone electrode. (Qualitative-one day).
6. Determination of composition and stability constant of Ferric-salicylic acid complex by Job's method. (Qualitative-two day).
7. Determination of critical micellar concentration(CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.

Reference books:

1. Practical Organic Chemistry, A. I. Vogel, ELBS, 2002.
2. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern, 1980.
3. Comprehensive Practical Organic Chemistry : Qualitative Analysis, V. K. Ahluwalia and S. Dhingra, Universities Press (India) Ltd, 2000.
4. N. K. Visnoi, Advanced organic Chemistry practical
5. D. P. Shoemaker, C. W. Garland and J. W. Niber, *Experiments in Physical Chemistry*,(1996) McGraw Hill Interscience.
6. Findlay's Practical Physical Chemistry, 9th Ed. Revised by B.P. Levitt, Longman.1973.
7. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
8. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).

PAPER – CHEM 805E
(Spectroscopic methods in inorganic Chemistry)
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit I:

Nuclear Magnetic Resonance Spectroscopy:

Basic principle, Relaxation time-spin lattice and spin–spin relaxation, Chemical shift, factors that affect chemical shift. Use of chemical shifts and spin-spin couplings for structural determination. Application of ^{1}H, ^{13}C, ^{19}F and ^{31}P in the structural assignment of selected inorganic compounds.

Electron Spin Resonance Spectroscopy:

Basic principle, the g-value and the factors affecting thereof; Hyperfine splitting (isotropic systems); interactions affecting electron energies in paramagnetic complexes (Zero – field splitting and Kramers degeneracy); Anisotropic effects (the g-value and the hyperfine couplings). Application of ESR spectra of simple free radicals, transition metal complexes (d^1 and d^9 ions in cubic and tetrahedral fields),anisotropic nature of g-values, hyperfine coupling constant, ESR spectra in structural assessment of inorganic compounds.

Unit II :

Infrared and Raman Spectroscopy:

Basic principle of IR and Raman spectroscopy; application of vibrational spectroscopy in investigating - Symmetry and shapes of simple AB_2, AB_3 and AB_4 molecules.

Structural elucidation (by IR & Raman spectra) of co-ordination compounds containing the common ligands such as: NH_3, H_2O, OH^-, $NO3^-$, $SO42^-$, ClO_4^-, CN^-, SCN^-, N_3^-, H^-, PR_3, OPR_3, halides, dioxygen, $-COO^-$, aminao acids.

Mass Spectroscopy:

Basic principle of mass spectrometry, concept of metastable ions and transitions, recognition of the molecular ion peak, Stevensan's rule.

Application to metal compounds containing ligand such as carbonyl/ nitrosyl/ alkyl/ cyclopentadienyl and acetyl acetonate. Interpretation of mass spectra for structural characterization. Effect of isotopes on the appearance of mass spectrum.

Mossbauer spectroscopy:

Principles, isomer shift, quadruple effect of magnetic field, application to iron and tin compounds.

Recommended Books:

1. R.S. Drago, Physical Methods for Chemists (1992), Saunders College Publishing, Philadelphia.
2. K. Nakamoto, Infrared Spectra of Inorganic and coordination compounds, 2nd Edn. 1970, Wiley-Interscience, London.
3. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication (Zeneca) 1997).

PAPER: CHEM 806E

X-ray Crystallography and solid state Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I

Crystals Lattices and symmetry: Definition of a crystal, Lattice points, Unit Cells, Unit Cell calculations; Definition of symmetry, Symmetry operations and elements of symmetry, Point groups, Classification of unit cells, Crystal systems, Herman-Mauguin notation, Bravais Lattices, Distinction between trigonal and hexagonal systems, Crystal planes and indices Law of rational indices. ***Space groups and equivalent positions:*** Screw axis, Glide planes, Space groups, Relationship between space groups, point groups, and physical properties, Equivalent positions, Special positions, Space group tables in International Tables for X-ray crystallography.

Unit II

X-ray diffraction*:* Periodicity and structural information, The diffraction grating, Diffraction of X-ray by crystals, The Laue equations, Bragg's Law, Generalization of Miller indices, Electron density function, Fourier series, Fourier expansion of electron density, Intensities of diffraction spots, The phase problem, Calculation of structure factors, Effect of thermal vibrations, Structure factors of centro-symmetric crystals, Friedel's law, Laue groups, Structure factors of sodium chloride

Determination of atomic positions*:* Solutions of structure factor equations, The Patterson function Heavy-atom methods, Isomorphous replacement, Superposition methods, Inequalities, Sayre-Cochran-Zachariasen relationship, Hauptman-Karle methods, Summary of phase-determining methods, Refinement, Description of procedure for X-ray structure analysis (NaCl and CsCl)

Unit III: Solid state Chemistry: Solid State Reactions: Types; sintering; nucleation; Factors influencing the reactivity of solids;Precursors to solid state reactions; Tammann and Hedvall mechanism; Wagner's Diffusion theory of reaction; Material transport in solid state reaction—counter diffusion, Kirkendall effect; Huttig's mechanism; Kinetic model: Reaction in powder compact, parabolic rate law, Jander'srate equation. Crystal Defects: Types of defects, thermodynamics of Schottky and Frenkel defect formation, Kroger-Vink notation for crystal defects Atomic theory of diffusion—self diffusion mechanism.

Recommended Books:

1. Introduction to Crystallography, Donald E. Sands, Dover Publications, INC. New York.
2. Crystal Structure Analysis for Chemists and Biologist, Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, Wiley VCH, 1994.
3. Crystal Structure Determination, William Clegg, Oxford University Press, 1998.
4. Structure Determination by X-ray Crystallography, Mark Ladd and Rex Palmer (September 30, 2003).
5. Crystal Structure Determination, Werner Massa (March 31, 2004).
6. Crystal Structure Analysis, Jenny Glusker and Kenneth Trueblood (August 1992).
7. A. R. West. *Solid State Chemistry and its Applications*, John Wiley (1998).
8. N. B. Hannay. *Solid State Chemistry*, Prentice-Hall (1979).
9. D. K. Chakraborty. *Solid State*, New Age International, New Deldi (1996)

PAPER - CHEM 807E

Chemistry of Biomolecules-I

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I:

Chemistry of amino acids and peptides: Introduction to amino acids, essential amino acids; nomenclature of α-amino acids;structures, properties and synthesis of natural and non-natural α-amino acids; application of amino acids as building block and chiral ligand in organic synthesis; peptides and peptide synthesis, different strategies in peptide synthesis, solid phase methods; sequencing of polypeptides; enzymatic cleavage of peptide bond; preliminary concept of protein and their structures; protein denaturation; biosynthesis of amino acids.

Unit II:

Chemistry of carbohydrates: Classification; structure, nomenclature, stereochemistry, conformation, reactions of monosacharides (isomerization, glycoside formation, hydrazones and osazones, alditols by reduction, oxidation and oxidative cleavage); protective groups for monosaccharides; synthesis of monosaccharide and disaccharides (sucrose, maltose, lactose); carbohydrate metabolism; role of sugars in biological recognition. Structure and function of sugar derivatives (deoxy, amino, branched chain sugars); Polysaccharides of biological importance, dextran, sialic acid

Recommended text and reference books:

1. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford.
2. G. C. Barrett and D. T. Elmore, Amino acids and peptides (2004), Cambridge University press.
3. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
4. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
5. Norbert Sewald and Hans-Dieter Jakubke,Peptides: Chemistry and Biology.. Wiley-VCH
6. Ward, Selectivity in organic synthesis (1999), Wiley-VCH, 1999.
7. T. W. Greene, Protecting groups in Organic synthesis (2000), Wiley-VCH, 2000.
8. Chemistry of Biomolecules : An Introduction, R. J. Simmonds, Royal Society of Chemistry, 1992.

PAPER - CHEM 808E

Medicinal Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I:

Drugs and drug design: Concepts of drugs, classification, analogues and pro-drugs, theories of action, assay and metabolism of drugs;

Drug design, theory of drug design, structure activity relationship (SAR), Quantitative structure activity relationship (QSAR); introduction to combinatorial synthesis in drug discovery; Development of new drugs, procedures followed in drug design and development.

Unit II:

Synthesis and uses of the following drugs of different pharmacological activities:

a) Antimalerials: Quinine, chloquine, Trimethoprim

b) Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.

c)Anti-inflammatory: Aspirin, Ibuprofen, Oxyphenylbutazone, Diclophenac, Indomethacin, coxib, celecoxib.

d) Antitubercular and antileprotic:Ethambutol, Isoniazide&Dapsone

e) Anaesthetics: Lidocaine, Thiopental.

f) Antihistamines: Phenobarbital, Diphenylhydramine.

g) Tranquilizers: Diazepam, Trimeprazine

h) Cardiovascular: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol

i) Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloraethamine, cyclophosphamide, Mephalan, uracils, mustards.

Unit II: Antibiotics: Preparation of semi synthetic penicillin, conversion of penicillin into cephalosporin, synthesis of chloramphenicol (diastereoselective and enantioselective) general account of tetracycline & macrocyclic antibiotics (no synthesis)

Recommended text and reference books:

1 A. Kar, Medicinal Chemistry, New Age publications
2 Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-A Molecular and Biochemical Approach, Oxford University Press.
3 Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
4 Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-HilI (2005).
5 S. S. Pandeya& J. R. Dimmock.Introduction to Drug Design, New Age International.(2000).
6 D. Lednicer. Strategies for Organic Drug Synthesis and Design, John Wiley (1998).
7 Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).

PAPER - CHEM 809E

Advanced group theory

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

GROUP THEORY – I:

The concept of groups; group multiplication tables and the rearrangement theorem; subgroups, classes and the related theorems; commutative groups (Abelian), cyclic group; isomorphism and homomorphism. Examples.

Molecular point groups (in Brief) , similarity transformation and the invariance of characters of matrices under such transformation, matrix representation of point groups; reducible, irreducible and equivalent and inequivalent representations; the great orthogonality theorem (no derivation) and its corollaries, character tables, construction of character tables in complex cases such as $D_{6h,}$ T_d etc; the group of Schrodinger equation; basis function for irreducible representation "projection" operator; direct product representation .

GROUP THEORY - II (Physical Applications):

Symmetry factoring of secular equations; LCAO -MO ,II bonding and Huckel's theory ;some examples: ethylene ,bengene ,Naphthalein. symmetry based "selection rules" for cyclization reaction (Woodward Hoffmannrule) Hybrid orbital and Molecular orbitals for AB_n -type molecules. Crystal field theory (CFT) Splitting of energy levels, and terms in a chemical environment. Determining the symmetry types of the normal modes;selection rule for fundamental (infra-red and Raman) vibrational transitions. Mutual Exclusion rule.

Reference books:

1. Chemical Application of Group Theory – F.A. Cotton,3rd edition, A Wiley Interscience publication
2. Group Theory and Quantum Mechanics, M.Tinkham, Tata McGraw Hill, publishing Ltd.
3. Group Theory and Chemistry, David M. Bishop, Clarendon Press Oxford.
4. Group Theory and its application to Physical Problem, M. Hamermeah, Dover publication.

PAPER - CHEM 810E

Surface Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

ADSORPTION ISOTHERM:

Thermodynamics of adsorption isotherm, Different adsorption isotherms, Adsorption at solid-liquid, liquid-gas, liquid-liquid interfaces, Effect of added electrolyte on the surface excess of ionic surfactants.

MIXED SURFACTANTS:

Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, counter ion binding in mixed surfactants.

SOLUBILISATION AND EMULSIFICATION:

Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions and applications.

Reference books:

1. N.K.Adams, *Physics and Chemistry of Surface,*
2. A.W.Adamson, *Physical Chemistry of surface,*
3. M.J.Rosen, *Surfactants and Interfacial Phenomena,* (1978) John Willey, New York.
4. Y.Moroi, *Micelles: Theatrical and Application Aspects,* (1992) Plenum Press, New York

SEMESTER – III

Semester - III

CHEM	901C	Inorganic Chemistry-III	04
CHEM	902C	Organic Chemistry-III	02
CHEM	903C	Physical Chemistry-III	02
CHEM	904C	Chemistry Project-I	04
		Elective	
CHEM 905E	Analytical and separation Techniques in Chemistry		02
CHEM 906E	Enzyme Chemistry		02
CHEM 907E	Bioinorganic Chemistry		02
CHEM 908E	Chemistry of Biomolecules - II		02
CHEM 909E	Polymer Chemistry		02
CHEM 910E	Quantum Chemistry - II		02

PAPER - CHEM 901C

Inorganic Chemistry - III

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credits: 04

Unit I: Kinetics and Mechanism of Inorganic Reactions

(a) Energy profile of a reaction, Labile and inert complexes, dissociative, associative and interchange mechanisms of ligand substitution reactions, ligand substitution reactions in square planar and octahedral complexes, the trans effect, mechanism of isomerization, acid & base hydrolysis and racemization of tris-chelate complexes, Ray-Dutta and Bailar twist mechanisms.

(b) Mechanism of electron transfer (redox) reactions: various types of electrons transfer reaction (inner and outer sphere reactions, complementary and non-complementary reactions), Marcus-Husch theory and its applications, stereochemical non-rigidity and fluxional molecules.

(c) Study of complexes in solution: Stability of a complex in solution, thermodynamic and kinetic stability of complexes, factors affecting thermodynamic and kinetic stability of complexes, stability constant, determination of composition and stability constants of complexes by modern methods, conditional stability constants and their importance. Study of polynuclear and mixed ligand complexes.

Unit II: Transition and Inner transition metal chemistry

(a) Chemistry of Platinum metals: Important compounds of Platinum metals, comparative study of Lanthanides and Actinides with reference to oxidation states, complex formation, magnetic properties, colour and spectral properties, Lanthanide shift reagents.

(b) Transition metal π-acid complexes: π-acid ligands (CO, NO, tertiary phosphine, arsine etc.), structure, bonding, synthesis and reactivity of complexes of CO, NO, tertiary phosphine, metal carbonyl hydrides.

Unit III: Electronic Spectra of Transition metal complexes:

Spectroscopic states: micro states, terms of d^n configurations, Selection rules, Orgel diagram, Correlation diagram, Tanabe-Sugano diagram, calculation of ligand field parameters (dq, B and β values), Band intensities and band width, Spectra of high spin octahedral and tetrahedral complexes for d^1-d^9 systems, charge transfer spectra, Application of electronic spectra for structural characterization of coordination compounds.

Unit IV

Cluster Compounds: 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. Polyhedral skeletal electron pair theory and Total Electron Count theory – Wades rules – Capping rule, Mingo's Rules (selected examples). Carbide Clusters.

Metal Halide clusters: Dinuclear, Trinuclear, Tetranuclear Metal-Metal systems – Edge sharing, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures, Quadruple bond, Structure and bonding in Octahedral halides of $[Re_2Cl_8]^{2-}$, $[Mo_6(Cl)_8]^{4+}$.

Boranes, carboranes, metalloboranes, metallocarboranes.

Reference book

1. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5th Edition, Wiley Interscience, N.Y
2. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
3. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
4. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
5. J. Huhee, E.A. Keiter, R.L. Keiter & O.K. Medhi-Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn..Pearson Education, 2007.
6. G.L. Miessler & D.A. Tarr-Inorganic Chemistry, 3rd Edn, Pearson Education, 2007.
7. Allan K. Brisdon-Inorganic Spectroscopic methods, Oxford.
8. Introduction to Ligand field Theory- B.N.Figgis

PAPER - CHEM 902C

Organic Chemistry - III

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Nuclear magnetic resonance spectroscopy for organic compounds

NMR sample handling and solvent for NMR study, chemical shift, internal standards, factors affecting the chemical shift, NMR shift reagents, coupling constant, spin-spin coupling – vicinal and geminal coupling, long range coupling – two bond coupling (2J) three bond coupling (3J), Karplus relationship, multiplicity of splitting and relative intensity of lines, spin decoupling, coupling constants. First order spectra- A_3X, AX and AMX systems. Second order spectra- AB and A_2B_2 systems; Nuclear overhauser effect (NOE), chemically induced dynamic nuclear polarization (CIDNP), introduction of ^{13}C NMR spectroscopy: Principle, instrumentation; multiplicity, proton –decoupling, off-resonance decoupling, noise-decoupling, ^{13}C chemical shifts values, DEPT and INEPT terminology; Two dimensional NMR spectroscopy: magnetic resonance imaging (MRI).Application of NMR in the structure elucidation of organic compounds.

Unit II: Mass spectroscopy for organic compounds

Introduction – basic theory, instrumentation and sample handling. Methods of generation of mass ions – electron impact (EI), chemical ionization (CI), electron spray ionization (ESI) and fast atom bombardment (FAB) techniques, TOF-MALDI and SELDI; Tandem mass spectroscopy, general mass fragmentation pattern of organic compounds, base peak, molecular ion, relative intensity, mass ions fragmentation, metastable ions, even electron rule, nitrogen rule, HDI, application of mass spectroscopy.

Unit III: Main group Organometallic Chemistry:

Introduction: Definition, a brief history of organometallic chemistry, importance of organometallic compounds as reagents, additive and catalyst. Organometallic chemistry of lithium, magnesium, zinc, copper, aluminium, cadmium and mercury: synthesis, structures and reactivity. Metal alkyls, aryls and hydrides: Stability, preparation and reactivity.

Applications of main group organometallics in organic synthesis:

Recommended Books:-

1. Spectroscopic identification of organic compounds (8^{th} edition). R.M. Silverstein and F.X. Webster, John Wiley & Sons, Inc (2014).
2. Spectroscopic methods in organic chemistry (sixth edition). D. H. Williams and I Fleming, Tata McGraw Hill (2005).
3. Organic spectroscopy (3^{rd} edition). William Kemp, MacMillan (1991).
4. Applications of Absorption Spectroscopy of Organic Compounds. J.R. Dyer. Prentice Hall (Digitized 2008)
5. Introduction to Spectroscopy (5^{th}Edn), Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan (2009)
6. Inorganic Chemistry G.L. Miessler& D.A. Tarr-, 3^{rd}Edn, Pearson Education, 2007.
7. Basic Organometallic Chemistry - Concepts, Syntheses and Applications by B. D. Gupta, A. J. Elias, Universities Press (2010).
8. Organometallic Chemistry: A Unified Approach by R. C. Mehrotra, Anirudh Singh, 2nd Edition, New Age International, Publication Year: 1991, reprint (2014).
9. Organolithium reagents, Jonathan Clayden,

PAPER - CHEM 903C

Physical Chemistry - III

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT – I: Statistical thermodynamics

Independent subsystems and distinguishability. Boltzmann distribution (nondegenerate and degenerate cases). Review of partition function: Thermal De Broglie wavelength. Partition functions for electronic, nuclear, rotational and vibrational degrees of freedom. Thermodynamic quantities in terms of partition functions. Entropy of ideal gas. Gibbs paradox. Equilibrium constants (ideal gas reaction) in terms of partition function.

The mathematical proof of the equipartition of energy principle. Specific heats of solids, fluctuations.

UNIT-I I: IRREVERSIBLE THERMODYNAMICS

Entropy of irreversible processes – Clausius inequality; entropy production and entropy flow, Rate of entropy production – generalized forces and fluxes (heat flow, chemical reactions, electrochemical reactions); Entropy production in open system; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; Stationary non-equilibrium states -states of minimum entropy production, Curie Prigogine principle.

UNIT II: NON EQUILIBRIUM THERMODYNAMICS

Non-equilibrium statistical mechanics: Random Processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.

Reference books:

1. C. Kalidas and M.V.Sanganarayana, Non Equilibrium Thermodynamics – Principles and application, Macmillan India (2002).
2. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Interscience (1960).
3. D. A.McQuarrie, *Statistical Mechanics,* (2003), Viva Books Pvt. Ltd. New Delhi.
4. M. C.Gupta, *The statistical Thermodynamics*,(1990), New Age International (P) Ltd. New Delhi.
5. M. Dole, Introduction to Statistical Thermodynamics

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PAPER - CHEM 904C

Chemistry Project- I

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credits: 04

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PAPER - CHEM 905E

Analytical and separation Techniques in Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Electrochemical techniques

Electrode processes and thermodynamics of cells: Introduction, Electrochemical Cells and reactions, Faradaic and nonfaradaic processes, nonfaradaic processes and the nature of the electrode solution interface, faradaic processes and factors affecting rates of electrode reactions, Basic electrochemical thermodynamics, formal potentials, reference electrodes, Liquid junction potentials. Currents in Polarography: Charging or condenser current, Migration current, Diffusion current, Ilkovic equation, influence of supporting electrolyte, limiting current measurements. Potential sweep methods: Introduction, reversible systems peak current and potential, totally irreversible systems peak current and potential, quasi reversible system, cyclic voltammetry.

Unit II: Atomic Emission-Absorption Spectroscopy and thermo analytical techniques

Flame Atomic Absorption Spectroscopy: Principles of atomic absorption spectroscopy, Radiation sources, Flame and electrothermal atomization, Limitations in atomic absorption, Interferences, Comparison of absorption spectrometry techniques-flame and graphite furnace, Quantitative Analysis, inductively coupled plasma-mass spectroscopy (ICP-MS).

Flame Atomic Emission Spectroscopy: Atomic emission, Principles of flame emission photometry, Limitations of flame emission photometry, Interference, Qualitative Analysis, Quantitative Analysis, Comparison of flame atomic emission and absorption spectroscopy. Excitation sources in atomic emission spectroscopy, ICP-AES spectroscopy.

Thermo-analytical Techniques: Thermo gravimetric analysis (TGA), differential thermo gravimetric analysis (DTA), differential scanning calorimetry (DSC), Thermometric titration (principle, technique and application)

Unit III: Chromatographic techniques:

Basic concept of chromatographic separation – adsorption and partition chromatography, theory and handling of different chromatographic techniques – column, thin-layer, and paper chromatography. Gas chromatography: Basic principle, basic equipment; types of column and their selection; detectors (FID, TCD, ECD, NPD); sample separation and applications. High performance liquid chromatography (HPLC): Instrumentation - basic equipment; pumping and injection system, column and its packing, normal and reverse phases; detectors, sample separation and application. Gel permeable (filtration) chromatography, Size exclusion chromatography, gel electrophoresis

Recommended books:

1. Electrochemical Methods: Fundamentals and Applications by Allen J. Bard & Larry R. Faulkner, 2nd edition, Wiley India, Copyright 2004, reprint (2006).
2. Principles of Polarography by R. C. Kapoor & B. S. Aggarwal, Wiley Eastern Limited, (1991).
3. A Text-book of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, by A.I. Vogel, 3rd Edition, The English language book Society and Longmans, Green & Co Limited, (1956).
4. Atomic Absorption Spectrometry by B. Welz, M. Sperling, 3rd Edition, Wiley-VCH (1999).
5. Vogel's Text Book of Quantitative Chemical Analysis (6th Edition), Prentice Hall (2000).
6. Principles and Practice of Modern Chromatographic Methods, (1st Edition), Robards, Jackson & Haddad, Academic press (1994).
7. Chromatographic Methods (5th Edn), A. Braithwaite, J.F. Smith, Kluwar Academic Publisher.

PAPER - CHEM 906E

Enzyme Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Enzymes and Mechanism of Enzyme Action: General aspects of enzymes; nomenclature, classification and specificity, isolation, purification and function of enzymes. enzyme specificity activesites, Mechanism of enzyme action: mechanism at active sites,Transition state theory, orientation and steric effect, acid base catalysis, strain or distortion.covalent catalysis, acid base catalysis, proximity and orientation effects, zymogen, multi enzyme complexes, enzyme technology.

Kinetics of enzyme action – Michaeli's-Menten equation, Different plots for determination of K_m and V_{max} and their physiological significance; Enzyme regulation & drug design, Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis.

Unit –II: Co-enzyme Chemistry: Definition, classification, sources, biological functions of coenzymes; cofactors as derived from vitamins; coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine Pyrophosphate, Pyridoxal phosphate, lipoic acid, tetrahydrofolic acid, flavin coenzyme and heme coenzyme. Structure and functions of thiamine, riboflavine, pyridoxine, biotin, Vitamin B -complex, tocopherol and ascorbic acid and Vitamin -D, NAD^+, $NADP^+$, FMN, FAD and vitamin B_{12}.

Application and enzyme catalytic organic reactions – Oxidation, reduction, isomerization, epimerization, hydrolysis, phosphorylation, acylation, methylation, decarboxylation, dehydration. Enzymatic hydrolysis of peptides (carboxy peptidase, trypsin, chrymotrypsin and Lys C);

Recommended Books:

1. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7th Edition. W H Freeman & Co (Sd). 2017.
2. Bioorganic and Bioinorganic and Supramilecular Chemistry. P.S. Kalsi, New Age International (Pvt. Ltd.) 2nd edition 2010.
3. Biochemistry, C.B. Power and G.R. Chatwal. Himalayan Publishing House. 4th edition 1999.
4. Instant notes on Medicinal Chemistry. G Patrick. Viva Books Pvt. Ltd. 1st edition 2002.

PAPER - CHEM 907E

Bioinorganic Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I

Calcium in Biology: Biochemical role of calcium, Storage and transport of calcium, Role of Ca^{2+} in muscle contraction, Blood clotting mechanism, Biological calcification.

Unit II

Metallo-proteins and Metallo-enzymes of Fe : Ferritin, Transferrin, bio–mineralization and Siderophores, Peroxidase, Catalase, Hemerythrin, Cytochromes, Cytochrome P-450, Iron sulphur proteins, Rubredoxins, Ferredoxins.

Unit III

Metallo-enzymes and proteins of copper and zinc : Blue-copper proteins, Ceruloplasmin, Hemocyanin, Cytochrome -c oxidase, Superoxide dismutase, Carbonic anhydrase, Alcohol dehydrogenase, Carboxy peptidase, Metallothionein, inter changeability of Zn and Co in enzymes.

Unit IV

Biochemical role of Co, Mo and Mn, : Biological nitrogen fixation, Vitamin B12, B12 coenzyme, Cobalamines, Xanthine oxidase, Sulphite oxidase, Nitrite reductase, Arginase, Mn-SOD, Chlorophyll, Photosystem I and II, cleavage of water.

Unit V

Metals in medicines: Toxicity of Hg, Cd, Pb, Cr, Be, Se, and As. Biological defence mechanism, Chelation therapy, Metals used for diagnosis and Chemotherapy, Pt- complexes as anticancer drugs, complexes of Au, Cu, Zn, As, Hg, as drugs.

Suggested Reading:

1. Bioinorganic Chemistry, Asim K. Das. Books & Allied Ltd, 2013
2. Bioinorganic Chemistry (Bertini, Ivano G, Harry B ,Lippard, S. J, Valentine, J.S.), University Science Books, CA, 1994.
3. J.A. Cowan, Inorganic Biochemistry: An Introduction, 2nd Edition, Wiley-VCH , 1997
4. R. P. Hanzlik, Inorganic Aspects of Biological and Organic Chemistry,, Academic Press, New York, 1976

PAPER - CHEM 908E

Chemistry of Biomolecules-II

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I: Classification of lipids, biological importance of fatty acids and lipids, even chain and odd chain fatty acids, essential fatty acids: ω-3and ω-6 fatty acids; Oxidation of fatty acids (alpha, beta, and omega): saturated and unsaturated;odd carbon atom and even carbon atom fatty acids; saturated and unsaturated fats, ketone bodies, fatty acid metabolism, biological membranes, lipid peroxidation, properties and function of lipid bilayers and liposomes; self association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.

Unit II: Structure and functions of prostaglandins, and thromboxanes; Ecosanoids and prostaglandins, Source, synthesis and biological activities of prostaglandins and thromboxanes (PGE_1,PGE_2, PGE_3,PGF_1, PGF_2,PGF_3,PGG_2,PGI_2, PGH_2, TXA and TXB), biosynthesis of prostaglandins, inhibition of prostaglandin synthesis.

Unit –III: Synthesis, stability, reactivity and rearrangement of macrocyclic compounds, synthesis of mucone, civetone, exaltone and their bioactivity.

Books recommended:

1. Chemistry of Biomolecules: An Introduction, R. J. Simmonds, Royal Society of Chemistry, 1992.
2. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7th Edition. W H Freeman & Co (Sd). 2017.
3. 2. Bioorganic and Bioinorganic and Supramilecular Chemistry. P.S. Kalsi, New Age International (Pvt. Ltd.) 2nd edition 2010.
4. 3. Biochemistry, C.B. Power and G.R. Chatwal. Himalayan Publishing House. 4th edition 1999.
5. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford. .
6. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
7. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
8. Norbert Sewald and Hans-Dieter Jakubke,Peptides: Chemistry and Biology.. Wiley-VCH
9. *Maitland, Jr Jones, Organic Chemistry (1998).*
10. *J. Hopkins, C.W McLaughlin, S. Johnson, M.Q Warner, D. LaHart, J.D Wright .Human Biology and Health.Michelle (1993). Prentice Hall.*
11. *J.E Vance, D.E Vance, Biochemistry of Lipids, Lipoproteins and Membranes. Amsterdam: Elsevier (2002).*

PAPER – CHEM 909E

POLYMER CHEMISTRY

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

UNIT-I:

Polymer and Characterisation:-Banz concepts of polymer science, Molecular forces and chemical bonding in polymers. Polymer solution and fractionation. Gel permeation Chromatography and molecular weight determination by viscometry, osmometry, light scattering and ultra centrifugation, molecular weight distribution curve.

UNIT-II:

Polymerization:- mechanism and kinetics of step growth and chain growth polymerization- radical, ionic and ring opening polymerization, copolymerization, polymerization techniques and polymer reaction, polymer structure and physical properties: configuration of polymer chain crystal structure of polymers: speciality polymers: Block copolymer, polymer colloids and biomedical polymers.

Unit III: Organic and inorganic polymer

Organic polymer: Manufacturing process, general properties, compounding and applications of SBR, Polyisoprene, Polybutadiene, Butyl rubber, Ethylene –propylene rubber, Neoprene rubber, Speciality rubbers: Silicon rubbers, Nitrile rubbers, Polyacrylic rubbers –Polyurethane rubbers – foam rubber

Inorganic polymers:

Classification of inorganic polymer, inorganic polymerisation reactions (addition, condensation and coordination polymerisation). Polysiloxanes, polysilanes, poly phosphazenes, polymeric sulfur. Syntheisis, structure, properties and application of coordination polymers & organometallic polymers.

Reference books:

1. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
2. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
3. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
4. G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
5. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
6. F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New York.

PAPER – CHEM 910E
QUANTUM CHEMISTRY-II
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Group A: QUANTUM MECHANICS

UNIT-I

Interpretation of wave function (probability density). Box normalization. Superposition principle and expansion theorem. Derivation of the expression of L_z in polar coordinate system.P_x, L_z and $\hat{H}$ operators are Hermitian: Proof. Unitary and projection operators. Some important theorems. Schmidt orthogonalization. Dynamical variables and operators, dynamical states. Expectation value and average value. Linear vector spaces in quantum mechanics. Completeness theorem. Equations of motion of classical mechanics (in brief). Poisson bracket and Dirac's version of Correspondence principle. Ehrenfest theorem. Constants of motion.

The Heisenberg Uncertainty relations (position and momentum, angle and angular momentum , time and energy relations) : proof. Commutability and compatibility. Complete set of commuting operators. Fourier transform. Wave packet. Momentum space wave function.

Angular momentum operators (single particle system). Step up and step down operators. Spin angular momentum operators. Angular momentum operators (many electron system) and their commutation with spin free Hamiltonian operator. coupling of angular momenta, L-S coupling and j-j coupling. Term symbols and spectroscopic states. Pauli spin matrices and anti-commutation relations.

UNIT-II

Time independent non-degenerate perturbation theory (RSPT). Application: ground state of He atom. Degenerate RSPT. Applications: Stark effect, normal and anomalous Zeeman effect.

Rayleigh- Ritz variation principle. Linear variation method. Applications: ground state energy of He atom, harmonic oscillator.

Time dependent RSPT (First order). Fermi-Golden rule. Born-Oppenheimer approximation(in detail). Antisymmetrized wave Function. Slater determinant and Pauli exclusion principle.

Reference books:

1. L.I. Schiff, *Quantum Mechanics*, Third Edition, McGRAW-HILL BOOK COMPANY, 1985.
2. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
3. B.H. Bransden & C.J. Joachain, *Physics of Atoms and Molecules*, Longmann Scientific and Technical, 1994.
4. B.H. Bransden & C.J. Joachain, *Quantum Mechanics*, Second edition, low price edition, PEARSON Education, First Indian Reprint, 2004.
5. J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesely Publishing Company.
6. Eugene Merzbacher, *Quantum Mechanics*,Wiley International Edition, 1970.

SEMESTER –IV

Semester – IV

Core (12 credits)

CHEM	1001C	Inorganic Chemistry-IV	04
CHEM	1002C	Organic Chemistry-IV	02
CHEM	1003C	Physical Chemistry-IV	02
CHEM	1004C	Chemistry Project-II	04

Elective

CHEM	1005E	Supra-molecular and Nano Chemistry	02
CHEM	1006E	Environmental and Green Chemistry	02
CHEM	1007E	Chemistry of Natural Products	02
CHEM	1008E	Photochemistry	02
CHEM	1009E	Computer Programming	02
CHEM	1010E	Statistical Mechanics	02

PAPER: CHEM 1001C

Inorganic Chemistry-IV

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credits: 04

Group A

Transition Metal–Carbon Bond

(a) Transition Metal–Carbon σ-Bond: Brief review of metal alkyl compounds; transition metalcarbene and transition metal-carbyne compounds; transition metal vinylidene and transition metal allenylidene compounds.

σ – bonded ligands : Metal alkyls, aryls and hydrides. Stability, preparation and reactivity.

Metal- carbonyls / Metal- phosphines / metal- nitrosyls / metal isocyanide: structures, reactivity and bonding.

Metal- carbenes, metal-carbynes, Fischer carbenes, Schrock carbenes , N-heterocyclic carbenes, olefin metathesis.

(b) Transition Metal-Carbon π-Bond: Cyclopropenyl cation as a ligand; C4R4 as a ligand (R = H, Me, Ph); Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene metal carbonyls, η6-arene-chromium tricarbonyl in organic synthesis.

π - bonded ligands: Metal-olefins, metal alkynes, metal-dienes, Metal-Cp Metal-Cp* complexes. Synthesis, structure, bonding and reactivity.

Group B

1. Catalysis Using Organometallic Compounds: Terminology in catalysis (Turnover, Turnover number, Turnover frequency or turnover rate, mole fraction, eantioselectivity, stereoselectivity, chemoselectivity, regioselectivity); Comparison of Homogenous and Heterogeneous Catalysis; Catalytic Hydrogenation of alkenes and related reactions: Hydrogenation catalysts, Catalytic cycle

of Wilkinson's catalyst, Catalytic asymmetric synthesis, the mechanism of asymmetric hydrogenation using a chiral catalyst.

2. Olefin Metathesis: Well-known olefin metathesis catalysts and their properties, synthesis of Grubbs' and Schrock catalysts, Mechanism of olefin metathesis, ring opening metathesis, cross metathesis, ring closing metathesis, ring opening polymerization metathesis, acyclic diene metathesis polymerization, enyne metathesis, comparison of catalysts, application of catalytic olefin metathesis.
3. Palladium catalyzed C–C coupling reactions: The Heek reaction, Suzuki-Miyaura coupling, Sonogashira coupling, Stille coupling, Kumada coupling, Negishi coupling.
4. Olefin polymerization and oligomerisation reactions: The Ziegler-Natta catalyst, site control and chain end control mechanisms, metallocene based catalysts, post metallocenes catalyst.

PAPER: CHEM 1002C

Organic Chemistry-IV

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I: Heterocyclic chemistry

Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; Basicity and aromaticity of heterocycles; Synthesis, properties and reactions (ring openings & heteroatom extrusion) of 3- membered heterocycles (aziridines, oxiranes and thiiranes), 4- membered heterocycles (azetidine, oxetanes and thietanes); Synthesis and reactivity of azoles (imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiazole& their benzo derivatives) and azines (6-membered heterocycles with two hetero atoms -pyridazines, pyrimidines and pyrazines), caffeine; theobromine and theophylline.

Unit III: Nucleic acid chemistry

Nucleic acids, nucleic acid bases, Purine and pyrimidine bases of nucleic acids, nucleosides and nucleotides, their structures and nomenclature, structures and functions of NADH, NADP and ATP, Structures of RNA and DNA; replication of DNA; base-pairing, double helical structure of DNA.

Recommended Books:

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Pearson Education.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductiion to the Heterocyclic Compounds, R.M. Acheson, John-wiely.
7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.
8. Medicinal Natural Products, A Biosynthetic Approach 3rd Edition, Paul M Dewick, John Wiley & Sons Ltd.
9. Organic Chemistry Volume 2: Stereochemistry and the Chemistry of Natural Products, I. L. Finar, Fifth Edition, ELBS.
10. R.T. Morrison and R.N. boyd, Organic chemistry, 6thedn, Prentice hall of India, New delhi, 2003.

PAPER: CHEM 1003C

Physical Chemistry-IV

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

UNIT – I

A. ELECTROCHEMISTRY–I: Activity in electrolytic solutions. Freezing point depression and the mean ionic activity coefficient. The Debye-Huckel theory for dilute ionic solutions (derivation) and correction for concentrated solutions Equilibrium in ionic solutions. Ion association.

B. ELECTROCHEMISTRY–II: Electrodics - The basic electrodic equation: Butler-Volmer equation, over potential, polarisable and non-polarizable interfaces; Faradaic and non -faradaic Currents, Over-potentials, aspects of deviation from equilibrium. Electrical conductance of solutions; The Debye Huckel Onsagar equation for conductance (derivation); Conductance at high fields and high frequencies, Conductance in non-aqueous solvents. Fuel Cells: H_2-O_2 cell, Air-H cell; Electricity producing cells: Na-S, Sb-S.

Numerical problems.

UNIT-II

C. BIO-PHYSICAL CHEMISTRY: Hydrophobic effect and self organising systems, structure and functions of proteins and nucleic acids and their stability. Structure and functions of cell membranes; Ion transport through cell membranes and nerve conduction; Multiple equilibria; stacking and cooperative interactions in biological systems. Muscle contraction; Techniques for study of structure and functions of proteins and nucleic acids.

D. CHEMICAL KINETICS-II: Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple; Bi-molecular reactions; Collision theory; Activated complex theory. Reactions in solutions: Diffusion controlled and activation controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength; Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed uni-molecular and bimolecular reactions; Applications in ammonia synthesis and oxidation of carbon-monoxide.

Reference books:

1. J.O'M, Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Vol.1&2 (1998), Plenum Press, New York.
2. K. J. Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
3. H. Eyring, S. H. Lin and S. M. Lin, *Chemical Kinetics* (1999), Jhon Willey, New York.
4. K. Zeemanski, *Thermodynamics*

PAPER: CHEM 1004C

Chemistry Project II

Total Marks: 100 (Projrct 70 + Internal Assessment 30)
Credits: 04

PAPER: CHEM 1005E

Supra-molecular and Nano Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit-I: SUPRAMOLECULAR CHEMISTRY

Concepts and Languages of supramolecular chemistry - Molecules, super molecules and supramolecular Chemistry; factors leading to strong binding (non-covalent interactions); molecular receptors – design and principles; Types of interactions between host and guest molecules; Thermodynamics of host-guest complexation; Enthalpy and entropy contributions, complexation free energies; Molecular recognition – factors involved; Molecular receptors – for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands and ionophores; Creation of rotaxanes and catenanes; Supramolecular catalysis- Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules; Catalysis with Cyclophane Type Receptors; Catalysis of Synthetic reactions; Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Various types of supramolecular devices.

Unit –II: NANO CHEMISTRY

Background to Nano-science Science and Technology - Implications for Physics, Chemistry, Biology and Engineering - Classifications of nanostructured materials - nano particles - quantum dots, Nanowires, nano-tubes – ultra – thinfilms – multilayered materials. Typical syntheses of nano particles, oxide nano tubes and fibres, metal nano particles; Length Scales involved and effect on properties: Mechanical, Electronic, Optical, Magnetic and Thermal properties.

Synthesis of nanoparticle: Bottom-up Synthesis -Top-down Approach: Precipitation, Mechanical Milling, Colloidal routes, Self-assembly, Vapour phase deposition, MOCVD, Sputtering, Evaporation, Molecular Beam Epitaxy, Atomic Layer Epitaxy, MOMBE.

Characterization of nano particles- X-ray diffraction technique, Scanning Electron Microscopy - environmental techniques, Transmission Electron Microscopy including high-resolution imaging, Surface Analysis techniques

Application of nano-structured material in organic synthesis, dendrimers, bucky balls and nano tubes (properties and applications), drug delivery systems; Nanotechnology for sustainability, Nanomedicine, Environmental, health, and safety issues

Suggested reading:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. A.S. Edelstein and R.C. Cammearata, eds., Nanomaterials: Synthesis, Properties and Applications, (Institute of Physics Publishing, Bristol and Philadelphia, 1996)
3. N John Dinardo, Nanoscale charecterisation of surfaces & Interfaces, Second edition, Weinheim Cambridge, Wiley-VCH, 2000
4. G Timp (Editor), Nanotechnology, AIP press/Springer, 1999
5. Akhlesh Lakhtakia (Editor) The Hand Book of Nano Technology, "Nanometer Structure", Theory, Modeling and Simulations. Prentice-Hall of India (P) Ltd, New Delhi, 2007.

PAPER: CHEM 1006E

Environmental and Green Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit – I: Environmental Chemistry (Credit – 01)

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, Ozone depletion, The green-house effect and Global warming, El-Nino phenomenon. Micro-organism in aquatic chemical reactions, Eutrophication, Re-cycle of waste-water in process industry, Treatment of sewage and reuse of water in industry and agriculture, microbiologically mediated redox reactions and Nitrogen transformation by bacteria. Water pollutants: Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity, DO, BOD, COD etc.); industrial and waste-water treatment; Chemical hazards, chemical disaters, pollution of environment-man made, industrial, natural disasters, environmental biochemistry, toxicological chemistry; analysis of water and waste water, solid wastes and air pollution-Photochemical smog, Auto exhausts, Acid-rains, Air-quality standards. Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

Unit – II: Green Chemistry (Credit – 01)

Definition, Concepts and basic principles of green chemistry, need of green chemistry, green chemistry as an alternative tool for reducing pollution, atom economy, less hazardous chemical syntheses, atom economy in rearrangements, addition and pericyclic reactions, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, Green synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology. Development of new methods for organic synthesis such as Green Synthesis: use of sonochemistry, use of ionic liquids, use of microwaves, bio-catalysis. Selection of solvent: i) Aqueous phase reactions ii) Reactions in ionic liquids iii) Solid supported synthesis iv) Solvent free reactions, Green catalysts: i) Phase transfer catalysts (PTC) and ii) Biocatalysts. Microwave and Ultrasound assisted green synthesis: Aldol condensation, Cannizzaro reaction, Diels-Alder reactions, Strecker synthesis, Willaimson synthesis and Dieckmann condensation.

Book Suggested:

1. *Handbook of Environmental chemistry*, Springer-Verlag, O. Hutzinger.
2. M. Bernhard, F.E. Brinckman & P.J. Sadler.*The Importance of Chemical Speciation in Environmental Processes*, Springer-Verlag,
3. L.J. Fristschen, & L.W. Gay, *Environmental Instrumentation*, Springer-Verlag,.
4. Real World Cases in *Green Chemistry*, ACS, M.C. Cann & M.E. Connelly.
5. P.T. Enastas and T.C. Williamson, Green Chemistry: Designing Chemistry for Environment, ACS,
6. *Green separation processes, methods and application*, Fonso, National Scientific Book Agency, Delhi-110053.
7. G.W. Vanloon, S.J. Duffer, *Environmental Chemistry* - A Global Perspective, (2000) Oxford University Press.
8. F.W. Fifield and W.P.J. Hairens, *Environmental Analytical Chemistry*, 2nd Edition (2000), Black Well Science Ltd.
9. Colin Baird, *Environmental Chemistry*, (1995) W.H. Freeman and Company, New York.
10. A.K. De, *Environmental Chemistry*, 4th Edition (2000), New Age International Private Ltd., New Delhi.
11. Peter O. Warner, *Analysis of Air Pollutants*, 1st Edition (1996), John Wiley, New York.
12. S.M. Khopkar, *Environmental Pollution Analysis*, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
13. S.K. Banerji, *Environmental Chemistry*, 1st Edition (1993), Prentice-Hall of India,New Delhi

PAPER: CHEM 1007E

Chemistry of Natural products

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT – I

General: Sources and types of natural products, method of isolation and structure elucidation, importance of natural products, biosynthesis of some common type of natural products – terpeneoids, steroids, flavonoids and alkaloids.

Chemistry of terpenoids, **steroid and hormones:** Terpenoids – sesquiterpenoids, diterpenoids with special reference to the isolation, structure and stereochemistry: alpha-santonin, Caryophyllene and isocaryophyllene, abietic acid and Gibberellic acid.

Steroids and hormones – Cholesterol, oestrone, progesterone, testosterone.

UNIT- II Alkaloids and Phenolics - Chemistry of quinoline, isoquinoline, phenanthrene and indole group of alkaloids - papaverine, cimchonine quinine, morphine, thebaine, codeine, reserpine with special reference to isolation, structure and stereochemistry. Plant phenolics with special reference to the general structures, reactions and synthesis of anthocyanins, anthocyanidins, flavones flavonols, isoflavones, chalcones, coumarins, quinines and tannins.

Reference books:

1. Organic Chemistry, I.L. Finar, volume 2, ELBS, 5th edition (1975).
2. Organic Chemistry. Morrison Boyd and Bhattacharjee, 7th edition (2013), Pearson.

PAPER: CHEM 1008E

Photochemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT- I : Physical processes of Photochemistry

Physical properties of excited molecules: Nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids. Polarised luminencence, non radiative intra-molecular electronic transition, internal conversion, intersystem crossing, crossing potential energy surface (Franck- Condon factor).

Photo-physical processes in excited state: Types of photophysical pathways, Radiation less transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation. Mechanism of quenching, energy transfer process (Forster dipole coupling), electron transfer phenomenon (Marcus theorem, Rehm Weller theorem), eximer.

Unit II: Inorganic photochemistry and organic photochemistry

Introduction to inorganic photochemistry, Ligand field states,L-F excited states, charge transfer states , L-M-C-T states, M-L-C-T states, Thexi (and Dosenco states), photochemical reactions, substitutions, redox reactions of Cr(III), Ru(II) and RU(III) complexes. Application (synthesis and catalysis, chemical actinometry, photochromism, sensitization). Laser: Basic principles, population-inversion, qualitative description of ruby and He-Ne lasers.

Organic photochemical process: Quantum yields, photosensitization and its uses. Photochemistry of olefins and carbonyl compounds, Norrish – I and Norrish – II type reactions, photo oxygenation and photo fragmentation, Paterno-Buchii reaction, Barton reaction, Di-π-methane rearrangement, Photo-cycloaddition and Photochemistry of arenes. Photochemistry in vision process.

Reference books:

1. K. K. Rohtagi-Mukherjee, *Fundamental of Photochemistry*,(1986) New Age International New Delhi.
2. J. G. Calvert and J. N. Pitts, Jr., *Photochemistry* (1966) John Wiley & Sons, New York.
3. R. P. Wayne, *Principles and Application of Photochemistry* (1988), Oxford University Press, Oxford.
4. N. J. Turro, *Modern Molecular Photochemistry*, (1991) Univ. Science Books, Sansalito.
5. J. F. L Lakowicz, *Principles of Fluorescence Spectroscopy*, 2nd Edn. (1999) Planum Publishers, New York.

PAPER: CHEM 1009E

Fortran and C, C+, C++ Programming

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

FORTAN programming F77:

FORTAN programming preliminaries; FORTAN constants and variables; Arithmetic Expressions. Input-output statements. Simple computer programmes. Control statements. The Do statements. Subscripted variables. Elementary Format Specifications. Logical Expression. Function and subroutines. Processing files in FORTRAN. Use of common statements. FORTAN 90, 95(Introduction).

UNIT-II

C, C+ , C++

PAPER: CHEM 1010E

Statistical Mechanics

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

Classical monatomic liquids-radial distribution function (RDF); Relating RDF with the thermodynamic properties; integral equations; Potential of mean force; the direct correlation function.

Statistical mechanical perturbation theory of liquids: theory and its application to derive van der Waals equation of state.

UNIT-II: Non-equilibrium statistical mechanics: Random Processes; Time-correlation functions;

Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.

Reference books:

1. B. J. Mcclelland, *Statistical Thermodynamics*
2. M. Dole, *Introduction to Statistical Thermodynamics*
3. M. C. Gupta, *The statistical Thermodynamics* (1990), New Age International (P) Ltd. New Delhi
4. Anrew Maczek, S*tatistical Thermodynamics* (1978), Oxford University Press Inc. New York
5. D. A. McQuarrie, *Statistical Mechanics* (2003), Viva Books Pvt. Ltd. New Delhi.

Tripura University
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HOD Chemistry <hod_chemistry@tripu

draft syllabus

3 messages

HOD Chemistry <hod_chemistry@tripurauniv.in>
To: Mahesh Kumar Singh <mkchem.singh@gmail.com>, Mahesh Kumar Singh <mksingh@tripurauniv.in>, Ranendra DuttaPurkayastha <rndp09@gmail.com>, Ranendu Nath <rknath1995@gmail.com>, RN DuttaPurkayastha <rndp@tripurauniv.in>, S Majumdar <smajumdar@tripurauniv.in>, Utpal Chandra De <ucd1972@tripurauniv.in>
Thu, Oct 8, 2020 a

Please send me back the edited version of the revised syllabus for compilation. We shall sit together tomorrow at 1 for finalisation.
HOD, Chemistry

Utpal Chandra De <ucd1972@tripurauniv.in>
To: HOD Chemistry <hod_chemistry@tripurauniv.in>
Cc: Mahesh Kumar Singh <mkchem.singh@gmail.com>, Mahesh Kumar Singh <mksingh@tripurauniv.in>, Ranendra DuttaPurkayastha <rndp09@gmail.com>, Ranendu Nath <rknath1995@gmail.com>, RN DuttaPurkayastha <rndp@tripurauniv.in>, S Majumdar <smajumdar@tripurauniv.in>
Thu, Oct 8, 2020 at

I will send it soon.
[Quoted text hidden]

Ranendra DuttaPurkayastha <rndp09@gmail.com>
To: HOD Chemistry <hod_chemistry@tripurauniv.in>, S Majumdar <smajumdar@tripurauniv.in>
Fri, Oct 9, 2020 at

Enclosed herewith the Revised Syllabus .
Prof. RNDP
[Quoted text hidden]

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109K

There was meeting on

30/08/2020.

06/10/2020.

09/10/2020

A Departmental committee meeting is held on 09/10/2020 at 1:00PM at the HOD's Chamber, Dept. of Chemistry to finalise the REVISED SYLLABUS.

Members Present:

1. Prof M.K. Singh —
2. Prof. R.K. Nath — 09/10/2020
3. Prof. R.N. Dutta purkayastha — 09/10/2020
4. Dr. U.C. De — 09.10.2020
5. Prof. S. Majumdar — 09/10/2020

Resolution: In continuation of DC meeting dated 30/09/2020 and 06/10/2020 regarding the revision of Syllabus the following resolution was adopted:

(1) Total Syllabus in chemistry (PG) will be of minimum 80 Credit comprising 72 credit from the Core course and 8 credit from compulsory elective (from computer Skill - II and Basic Statistics) needs to be taken by the Students. The said compulsory elective to be adopt in their 1st Semester course.

(2) Students will be offered for Departmental elective courses in 2nd and 3rd Semester courses and the credit earned by the Students will be extra credit in addition of their minimum 80 credit.

(3) As the Chemistry project is included in the 4th Semester of his course therefore no elective course will be offer in 4th Semester programme. Two project papers of 50 marks and 100 marks of total 6 credit will be offered as core.

Prof. S. Majumdar
09/10/2020
Head, Dept. of Chemistry
Tripura University
Suryamaninagar-799022

TRIPURA UNIVERSITY
SURYAMANINAGAR 799 022
CHOICE BASED CREDIT SYSTEM (REVISED 2020)*

Course Curriculum – M. Sc. in Chemistry, Tripura University

Course Code	Name of the Courses	Marks	Credits
Semester –I (18 Credits core)			
CHEM 701C	Inorganic Chemistry-I	100	04
CHEM 702C	Organic Chemistry-I	100	04
CHEM 703C	Physical Chemistry-I	100	04
CHEM 704C	Chemistry Practical-I	150	06
Compulsory Elective (8 credits)			
CHEM 704E	Basic Statistics	100	04
CHEM 705E	Computer Skill II	100	04
Semester – II (18 Credits core)			
CHEM 801C	Inorganic Chemistry-II	100	04
CHEM 802C	Organic Chemistry-II	100	04
CHEM 803C	Physical Chemistry-II	100	04
CHEM 804C	Chemistry Practical-II	150	06
Elective			
CHEM 805E	Bio-inorganic Chemistry	50	02
CHEM 806E	Bio-organic Chemistry	50	02
CHEM 807E	Surface Chemistry	50	02
CHEM 808E	Quantum Chemistry	50	02
Semester – III (18 credits core)			
CHEM 901C	Inorganic Chemistry-III	100	04
CHEM 902C	Organic Chemistry-III	100	04
CHEM 903C	Physical Chemistry-III	100	04
CHEM 904C	Chemistry Practical-III	150	06
Elective			
CHEM 905E	Special topics in chemistry	50	02
CHEM 906E	Chemistry of natural products	50	02
CHEM 907E	Environmental and green chemistry	50	02
CHEM 908E	Advanced group theory	50	02
Semester – IV (18 Credits core)			
CHEM 1001C	Inorganic Chemistry-IV	100	04
CHEM 1002C	Organic Chemistry-IV	100	04
CHEM 1003C	Physical Chemistry-IV	100	04
CHEM 1004C	Chemistry Project – I	50	02
CHEM 1005C	Chemistry Project – II	100	04

09/10/2020
Prof. S. Majumdar
Head, Dept. of Chemistry
Tripura University
Suryamaninagar 799022

09/10/2020

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09/10/2020

DEPARTMENT OF CHEMISTRY
TRIPURA UNIVERSITY
SURYAMANINAGAR 799 022
CHOICE BASED CREDIT SYSTEM (REVISED 2020)*

SEMESTER I

INORGANIC CHEMISTRY - I
PAPER – CHEM 701C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 04

Unit-I - Symmetry and Group Theory: 12L

Symmetry elements and operations, equivalent symmetry elements and equivalent atoms, point groups with examples, Group of very high symmetry, systematic procedures for symmetry classification of molecules and illustrative examples, molecular symmetry for compounds having coordination number 2 to 9, molecular dissymmetry and optical activity.

Brief representation of theory of groups, matrix representation of groups, reducible and irreducible representation of point groups, definition of classes and character, the "Great Orthogonality Theorem", character tables, concept of character projection operator, normal modes of vibrations, symmetry of normal vibration, selection rules for IR and Raman Transitions.

Unit-II – Stereochemistry and Bonding: 12L

Brief review of the Periodic properties, ionic bonding, electronegativity (Pauling, Mulliken and Allred-Rochow methods); review of VSEPR model and the use of outer d-orbitals.

Valence bond theory,hybridization**,** dπ-pπ bond; LCAO-MO theory for homo-nuclear diatomic molecules; hetero-nuclear diatomic molecule; polyatomic molecules; orbital symmetry and overlap; molecular shapes in terms of molecular orbitals; Walsh Diagrams, non-covalent interactions.

Unit III- Spectroscopy –I 12L

Infrared and Raman Spectroscopy: Brief review of basic principles of IR and Raman spectroscopy; application of vibrational spectroscopy in investigating - Symmetry and shapes of simple AB_2, AB_3 and AB_4molecules.Structural elucidation (by IR & Raman spectra) of co-ordination compounds containing the common ligands such as: NH_3, H_2O, OH^-, NO^{3-}, SO_4^{2-}, ClO_4^-, CN^-,SCN^-,N_3^-, H^-, PR_3, OPR_3, halides, dioxygen, $-COO^-$.

Mass Spectroscopy: Basic principle of mass spectrometry, concept of metastable ions and transition, recognition of the molecular ion peak, Application to metal compounds containing ligand such as carbonyl/ nitrosyl/ alkyl/ cyclopentadienyl and acetyl acetonate; Interpretation of mass spectra for structural characterization; Effect of isotopes on the appearance of mass spectrum.

Mossbauer spectroscopy: Principles, isomer shift, quadruple effect of magnetic field, application to iron and tin compounds.

Unit IV - Basic Bioinorganic Chemistry: 12L

Essential elements in biological system ,inorganic elements in biological systems, basic bioenergetics, Structure and function of biological membranes, active transport of cations across membrane, Crown either complexes of Na and K, Ionophores, Sodium /Potassium pump; Metalloporphyrins, heam proteins –haemoglobin and myoglobin: structure, thermodynamics and kinetics of oxygenation.

Recommended Books:

1. J. E. Huheey, E. A. Keiter, R. L Keiter and O. K. Medhi. Principles of Structure and Reactivity. First impression, Pearson Education 2006.
2. F. A. Cotton. Chemical Applications of Group Theory (3rd Edn) John-Wiley and Sons.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry (5th edition) John Wiley

4. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, Shriver and Atkins Inorganic Chemistry, Oxford University Press (2006).
5. Bioinorganic Chemistry, Asim K. Das, Books& Allied Ltd, 2013.
6. R. S. Drago, Physical Methods for Chemists (1992), Saunders College Publishing, Philadelphia.
7. K. Nakamoto, Infrared Spectra of Inorganic and coordination compounds, 2nd Edn. 1970, Wiley-Interscience, London.
8. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication(Zeneca) 1997).
9. Bioinorganic Chemistry (Bertini, Ivano; Gray, Harry B.; Lippard, Stephen J.; Valentine, JoanSelverstone), University Science Books, CA, 1994.

ORGANIC CHEMISTRY –I

PAPER: CHEM 702C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

Unit I: Organic reaction mechanism 12L

Structure and reactivity of organic molecules, aromaticity, annulenes; Concept of hard and soft acids and bases, isotope effects for determination of reaction mechanisms, Linear free energy relationship; Hammett equation, σ–ρ relationship, non-classical carbenuim ion (or carbocation), kinetic and thermodynamic control, transition states and intermediates, Hammand principle, Curtin-Hammett principle,. General reaction mechanism, aliphatic substitution reaction, SN1, SN2, mixed SN1 and SN2 and SNi reaction, SET reaction, electrophilic substitution reaction, SE1, SE2, SEi mechanism, electrophilic and nucleophilic aromatic substitution reaction, SNAr, SRN1 mechanism, reactivity, effect of substrate, leaving group and attacking nucleophile, elimination reaction, E1 E2 and E1Cb.

Unit II: Stereochemistry 12L

Chirality and isomerism in organic compounds, interconversion of Fischer, Newman and Sawhorse and Flying-wedge formula, *R-S* nomenclature,conformational analysis of cyclic compounds such as substituted cyclohexanes, fused ring systems (decalins, PHA, PHP), symmetry elements and point groups, axial and planar chirality, axial dissymmetry and centro dissymmetry, atropisomerism, stereochemistry of allenes, biphenyls and spiro compounds. Topicity, allylic strains, alkylketone effects, haloketone rule, methods of asymmetric synthesis, enantio-, and diastereo selective synthesis, determination of enantiomeric and diastereomeric excess, methods of resolution, stereospecific synthesis, effect of conformation on reactivity, optical purity, optical activity in absence of chiral atom.

Unit III: Reactive intermediates -I 12L

Structure, reactivity and stability of carbocations, carbanions, carbenes and nitrenes; classical and nonclassical carbocations; mechanism of condensation reactions involving enolates- Aldol, cross Aldol, Knoevenagel, Claisen, Perkin, Favorski and Stobbe reactions. Rearrangement reactions involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement, Demjenov rearrangement, dienone-phenol rearrangement), carbenes (Wolff & Arndt- Eistert synthesis), cyclopropanation, Simon-Smith reaction, rearrangement involving electron deficient nitrogen (Hoffman, Curtius, Schmidt, Lossen, Beckman), and oxygens (Bayear Villiger oxidation, cumene hydroperoxide), PPA cyclization and Fries rearrangement.

Unit IV: Reactive intermediates - II **12L**

Arynes: Generation, structure and stability; Benzyne mechanism for aromatic nucleophilic substitution; Rearrangement and cyclo-addition reactions of arynes, synthetic applications.

Enamines: methods of preparation, structure and stability of enamines; selectivity in the synthetic applications.

Free radicals: Generation, structure and stability of radicals, radical- initiator, scavenger substitution and addition reactions involving radicals, tributyl tin hydride mediated radical reactions, exo- and endo cyclisation and applications

Recommended text and reference books:

1. F. A. Carey and R. J. Sundberg. Advanced Organic Chemistry. 5thEdn. Plenum. Part – I, Part – II.
2. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4thedn, John Willey
3. R.T. Morrison and R.N. Boyd, Organic chemistry, 6thedn, Prentice hall of India, New Delhi, 2003.
4. Michael B. Smith & Jerry March, Advanced Organic Chemistry Reactions, Mechanisms, and Structure. (2013) Wiley-Interscience.
5. D. Nasipuri, Stereochemistry, Conformation and mechanism, 2ndEdn. John Wiley
6. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 2007.
7. S. Sengupta Basic Stereochemistry of Organic Moleclules, Book Syndicate Pvt. Ltd. 2nd Edn.
8. P.S. Kalsi, Stereochemistry, Conformation and Mechanism, 8th Edition. New Age Int., 2015.
9. T. Laue and A. Plagens, Named OrganicReactions,2nd edition (2005), John Wiley & Sons Ltd**.**
10. Reinhard Bruckner Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
11. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press.
12. A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.
13. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, John Wiley & Sons Inc. 5th Edition.
14. W. Carruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University Press (2004).
15. H. O. House, Modern Synthetic Reactions, 3rd Edition (1992), Benjamin Publishing Co.

PHYSICAL CHEMISTRY - I

PAPER: CHEM 703C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

Unit –I: Quantum Mechanics: **12L**

General Principles of Quantum Mechanics

Introduction; linear operators; Hermitian operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; separability of Schrodinger equation ; equation of motion.

Application to Simple Systems and Approximation Methods

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential, tunnelling effect and hydrogen atom. Antisymmetry principle and many-electron wave finctions.

Chemical Bonding

Born-Oppenheimer approximation (Introduction); valence bond (VB) theory and molecular orbital (MO) theory for diatomic molecules – hydrogen molecule ion, hydrogen molecule; excited states of H_2 – singlet and triplet; non-crossing rule and correlation diagram.

Unit -II: Kinetic Theory and Transport Properties of Gases: 12 L

Derivation of Maxwell's distribution of molecular speed**;** The general equation for transport, Thermal conductivity of gases, Molecular collisions and mean free path, Viscosity of gases, Diffusion , Introduction to the concept of non-steady state, Numerical problems.

Unit -III: Spectroscopy-I 12 L

Rotational(microwave)spectra, rigid diatomic molecule, Energy expression; Rotational constant. Selection rules. Determination of bond length from observed rotational spectra. Spectral intensity-degeneracy of rotational energy levels and total relative population.The effect of isotopic substitution.Non-rigid rotator (energy expression only).Chemical analysis by microwave spectroscopy.

Vibrational (infra-red) spectra:Simple harmonic oscillator model. Corresponding selection rule.Anharmonic oscillator model-Morse function.Selection rules.Fundamental absorption and overtones.Hot bands. P-,Q-,R- branch in IR spectra. IR spectra of linear molecules.Parallel and perpendicular vibrations.Chemical analysis by IR techniques.

Raman spectroscopy: Rayleigh scattering and Raman scattering (classical and quantum mechanical consideration). Stokes and Anti-stokes lines.Selection rule.O- and S-branch in Raman spectra.Rotational Raman spectra of homonuclear diatomic molecules.Vibrational Raman Spectra .The rule of mutual exclusion.Structure determination from Raman and IR spectra.

Numerical problems.

Unit -IV: Chemical Kinetics-1: 12 L

Opposing and consecutive reactions, complex reactions, Atomic and free radical chain reactions. Kinetic salt effect; Effect of solvent on rate constant (Single sphere and double sphere model): Non-Arrhenius equations and its significance. Theory of absolute reaction, rate (statistical) and comparison with that of collision theory;Kinetics of enzyme reaction (effect of pH) Michaels- Menton Law, derivation; Numerical problems

Suggested reading:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. D.A.MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
3. A.K.Chandra, *Introductory Quantum Chemistry*, 4th Edition, Tata McGraw Hill, 1997.
4. Levine, *Quantum Chemistry*, (1994)Tata McGraw Hill, New Delhi.
5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, (1935), McGraw Hill, New York.
6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
7. D. A. McQuarrie and J.D. Simon, *Physical Chemistry*, VIVA Students Ed. (2003)
8. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill International Edition
9. C. N. Banwell, E. M. McKash; Fundamentals of Molecular Spectroscopy, Tata McGraw Hill.
10. K.J.Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
11. H.Eyring, S.H. Lin and S.M.Lin, *Chemical Kinetics*, (1999)Jhon Willey, New York.
12. G. L. Agarwal; Basic Chemical Kinetics, Tata McGraw-Hill.

LABORATORY COURSE-I

PAPER: CHEM 704C (Inorganic Chemistry)

Total Marks: 100 (Practical 105 + Internal Assessment 45)

Credit: 06

1. Semi micro qualitative analysis of Inorganic salt mixtures containing (06) six radicals including W, Mo, V, Ti, U, Th, Zr, Ce and at least one interfering radical ($F^-/PO_4^{3-}/BO_3^{3-}$, CrO_4^{2-}).
2. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three component mixtures and alloys.
3. Preparation of the following inorganic compounds and characterization by IR, UV-Visible, Conductance & magnetic susceptibility measurements.
   (a) Tris (acetyl acetonato)manganese (III)
   (b)Tris (acetyl acetonato)iron (III)
   (c) Bis (acetylacetanato) oxovanadium(IV)
   (d) Renkei's Salt
   (e)Linkage isomer of nitro &nitridopentammine Cobalt (III) Chloride
   (f)Tris (Ethylenediammine) Nickel (II) Chloride. Dehydrate

Suggested Books

1. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas. Vogel'sTextbook of Quanti-tative Chemical Analysis, Peterson Education (2000).
2. G. Marr& B. W. Rockett. Practical Inorganic Chemistry, Van Nostrand (1972).
3. G. Pass& H. Sutcliffe. Practical Inorganic Chemistry (2nd edn.), Chapman & Hill (1974)
4. G. Brauer, Ed., Handbook of preparative Inorganic Chemistry, Academic Press, Vol 2, 1965,

Compulsory Electives

BASIC SATISTICS

PAPER – CHEM 704E

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

Syllabus: to be provided by Dean office/Department of Statistics

COMPUTER SKILL II

PAPER – CHEM 705E

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

Applications of Computer. Binary Number System: Conversion of binary number into decimal form, Conversion of decimal number into binary form, addition of two binary numbers, multiplication and division, Subtraction of two binary numbers using two's complement. Octal number system: Conversion of octal number into decimal form, Conversion of decimal number into octal form, Conversion of binary number into octal form, Conversion of octal into binary form, Hexadecimal number system: Conversion of Hexadecimal number into binary form, Conversion of binary number into hexadecimal form, Conversion of hexadecimal number into decimal form. Basics of algorithms and Flow chart: Key features of Algorithms: Sequence, decision and repetition. Flowcharts: significance of flowcharts, advantages and limitations. Basics of Programming language Introduction to C: Keywords, identifiers, variables, constants, input/output statement in C, operators in C, decision control and looping statements, arrays and strings. Computation with spreadsheet: Data management using excel-sorting, filtering, validation, Basic functions, logical functions, mean, mode, median, standard deviation, correlation, Chart

SEMESTER II

INORGANIC CHEMISTRY - II
PAPER – CHEM 801C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 04

Unit I – Spectroscopy-II: 12L

Nuclear Magnetic Resonance Spectroscopy - Basic principle, Relaxation time-spin lattice and spin–spin relaxation, Chemical shift, factors that affect chemical shift. Use of chemical shifts and spin-spin couplings for structural determination. Application of ^{1}H, ^{13}C, ^{19}F ,^{31}P and ^{119}Sn in the structural assignment of selected inorganic compounds.

Electron Spin Resonance Spectroscopy - Electron Paramagnetic Resonance Spectroscopy: Principle, instrumentation, representation of EPR spectrum, X-band and Q-band spectra, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: expected number of lines, intensities. Spectra of transition metal complexes(d^{1} -d^{9} ions in cubic and tetrahedral fields) , metal hyperfine anisotropic spectra, zerofield splitting, Kramers degeneracy, application: determination of oxidation state of metal ion in samples

Unit II -Magneto-chemistry: 12L

Different types of magnetic behaviour of materials and their origin, magnetic susceptibility and magnetic moment, measurement of magnetic susceptibility (Gouy and Faraday methods), Derivation of Curie equation for magnetic moment, Curie and Curie-Weiss law, quenching of orbital moments, Magnetic behavior of multi-electron system, orbital coupling, spin-coupling, spin-orbit coupling (RusselSaunder's coupling), spin-orbit coupling constant, j-j coupling, micro-states and term symbols, Lande interval rule, Thermal energy and magnetic moment, anti-ferromagnetism and its exchanged pathways.

Unit III -Coordination Chemistry: 12L

Brief review of theories of coordination compounds (VBT, CFT), Ligand Field Theory (LFT), Electronic absorption spectra of octahedral and tetrahedral complexes, Orgel diagrams, Tanabe- Sugano diagrams, calculation of Dq, B and ß values, selection rules, band intensities and band widths, spectra of high spin octahedral and tetrahedral complexes of d^{1} to d^{9} systems, Spectrochemical series; Adjusted crystal field theory, Nephelauxetic series, Tetragonal distortion, Jahn-Teller effect, Molecular orbital theory of complexes (including complexes with and without π bonding), MO diagrams for octahedral and tetrahedral complexes, Charge-transfer spectra.

Unit IV -Analytical Chemistry: 12L

Thermoanalytical methods - Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Electrochemical methods - Coulometry, Polarography, cyclic voltammetry, electrogravimetry.

Atomic Emission-Absorption Spectroscopy- Flame Atomic Absorption Spectroscopy: Principles of atomic absorption spectroscopy, Radiation sources, Flame and electrothermal atomization, Quantitative Analysis, Flame Atomic Emission Spectroscopy: Atomic emission, Principles of flame emission photometry, , Qualitative Analysis, Quantitative Analysis.

Suggested reading:

1. Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn. J. Huhee, E.A. Keiter, R.L.Keiter& O.K. Medhi Pearson Education, New Delhi.
2. Shriver & Atkins - Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
3. R. L. Dutta and A. Syamal, Elements of Magnetochemistry (2ndEdn), EWP (2010)
4. J. D. Lee, Concise Inorganic Chemistry (5thEdn) John Wiley & Sons (1996).
5. R.S. Drago, Physical Methods for Chemists(1992), Saunders College Publishing, Philadelphia.
6. J. A. Iggo, NMR Spectroscopy in Inorganic Chemistry, OUP Oxford (2000)
7. Fundamental Concepts of Inorganic Chemistry, Vol.7, Asim.K.Das & Mahua Das, CBS Publishers & Distributors, Pvt. Ltd., New Delhi, 2014.
8. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication(Zeneca) 1997).
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, New Age international Ltd, Publishers, New Delhi.\
10. A Text-book of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, by A.I. Vogel, 3rd Edition, The English language book Society and Longmans, Green & Co Limited, (1956).

ORGANIC CHEMISTRY –II
PAPER: CHEM 802C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 04

Unit I: Strategies and reagents in organic synthesis 12L

Designing of organic synthesis - Retrosynthetic and Disconnection approach; Reversal of dipoles (umpolung of reactivity) and it's applications; Synthons and retrons, linear and convergent synthesis, protection and deprotection strategies for common functional groups in organic synthesis; Applications of crown ether and phase transfer catalyst. Uses of the following reagents in organic synthesis: IBX, Dess-Martin periodinane, chloranil, DDQ, K-selecteride and L-selecteride, sodium cyanoborohydride, super hydrides, 9-BBN, Mukaiyama reagent, LDA, dicyclohexylcarbodimide, Corey-Nicolaou reagent, baker's yeast, CBS reagents.

Unit –II: Unit II: Orbital symmetry reaction 12L

Orbital symmetry, electrocyclic, cycloaddition, sigmatropic and group transfer reactions; Woodward-Hoffmann rule in pericyclic reactions; Rationalization based on FMO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Chelatropic reactions, 1,3-dipolar cycloaddition Cope, aza-Cope, oxy-Cope, Claisen, Somelett-Hauser rearrangements.

Photochemistry: Cis-trans isomerisation, Paterno-Buchi reaction, Norrish type I & II reaction, photoreduction of Ketones, di-pi-methane rearrangement, photochemistry of arenes, Photo-Fries rearrangement of ethers and anilides; Hoffmann-Loeflller-Freytag Reaction, Barton reaction.

Unit III: Oxidation and reduction reactions of organic compounds: 12L

Oxidation: Oxidation by Cr and Mn compounds; oxidation of alcohol, aldehyde, C=C, C-H bonds, PCC, oxidation with per acids and peroxides, ceric ammonium nitrate, Thallium(III) nitrate, Prevost and Woodward hydroxylation, cis- and trans- hydroxylation, glycol cleavage reagents: $KMnO_4$, OsO_4, HIO_4, $Pb(OAc)_4$, mercuric acetate, SeO_2 oxidation of allylic C-H bond. Epoxidation of alkenes- Sharpless epoxidation.

Reduction: Catalytic hydrogenation and dehydrogenation, dissolving metal reduction, reduction of functional groups, Meerwein-Pondrof-Verley reduction, hydroboration and related reaction, reaction of alkyl borane, Wolff-Kishner reduction, non-metallic reducing agents such as diimide.

Unit IV: Selective named reactions 12L

Swern oxidation, Moffat oxidation, Henry reaction, Wittig reaction and Horner-Wordwoth-Emmons reaction (stabilized and non-stabilized ylide); Nazarov cyclization, Pictet-Sprengler reaction, Passerini reaction, Ugi reaction, Peterson's synthesis, McMurry olefination, Julia olefination, Shapiro reaction, Chichibabin reaction, Baylis-Hillman Reaction, Staudinger Reaction.

Suggested reading:

1. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press.
2. A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.
3. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, John Wiley & Sons Inc.
4. W. Carruthers, *Some Modern Methods of Organic Synthesis,* Cambridge University Press
5. T. Laue and A. Plagens, Named OrganicReactions,2nd edition (2005), John Wiley & Sons Ltd**.**
6. H. O. House, Modern Synthetic Reactions, 3rd Edition (1992), Benjamin Publishing Co.
7. S. Warren, Organic Synthesis, Disconnection Approach, 1982, Wiley Interscience, NY
8. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry Part A and Part B.
9. T. Laue and A. Plagens, Named Organic Reactions,2nd edition (2005),John Wiley & Sons Ltd
10. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4thedn, J. Willey
11. R.T. Morrison and R.N. Boyd, Organic chemistry, 6thedn, Prentice hall of India, New
12. B. Dinda, Essential of Pericyclic and organic photochemistry, Springer (2016).
13. J. Sing & J Singh, Photochemistry and pericyclic reactions, New Age International (Pvt. Ltd). 3rd Edition (2010).

PHYSICAL CHEMISTRY - II

PAPER – CHEM 803C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Unit-I: Chemical Thermodynamics 12 L

Nernst heat theorem and the third law of thermodynamics, Calculation of entropy changes in chemical reactions, Mathematical and thermodynamic probability. Entropy and probability.The free energy of a mixture.Dependence of thermodynamic functions on composition.Partial molar quantities.

Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures.Concept of fugacity.

Analytical form of the chemical potential in ideal solutions.Chemical potential of the solute in a binary solution Application of Gibbs-Duhem equation.

The concept of activity:the rational concept and the practical concept. Colligative properties and activity of solute. Activities and reaction equilibria, experimental determination of activity coefficients of non-electrolytes, Numerical problems.

Unit -II : Adsorption and Aggregation: 12 L

Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation; Adsorption in liquid systems: Gibbs adsorption isotherm; Adsorption on solids: Langmuir isotherm, BET isotherm.

Surfactants, classification of surfactants, hydrophobic interaction, aggregation/micellization of surfactants, critical micelle concentration (cmc), factors affecting the cmc, thermodynamics of Micellization: phase separation and mass action models. concentration (CMC) of surfactants, thermodynamics of micellization. General experimental techniques employed in surfactant studies like tensiometry,conductometry, viscometry, spectrophotometry.

Brief introduction to soaps and detergents, their performance in soft and hard water conditions

Unit -III: Spectroscopy –II 12 L

NMR Spectroscopy: Theory for NMR Population of energy levels. Larmor precession. Relaxation times: spin - lattice relaxation, spin-spin relaxation. Fourier transform spectroscopy in NMR .Chemical shift.Shielding and de-slielding mechanism.Fine structure, spin-spin splitting, coupling constant.Strongly coupled systems, shift reagent in NMR.Hyperfine structure. Nuclear overhauser effect (NOE), 1H and ^{13}C NMR. Two-Dimentional NMR.Chemical analysis by NMR techniques.

ESR Spectroscopy : General background of ESR spectroscopy .Representation of ESR spectrum. 'g' - value, ESR spectra of simple organic free radicals; Hyperfine coupling, prediction of expected number of lines and their relative intensities, ESR spectra of transition metal complexes, metal- hyperfine coupling, anisotropic ESR spectra, zero field splitting, application of ESR spectroscopy examples.

Unit -IV: Spectroscopy –III 12 L

***Photoelectron Spectroscopy (PES)*:**Frank- Condon principle, Basic principles of photoelectron and X-ray photoelectron spectroscopies and their applications for chemical analysis of surfaces; application of ESCA and Auger spectroscopy for the studies of solids.

NQR: Nuclear quadruple resonance, Energy levels of a nucleus in a non-uniform electric field. Quadruple coupling constant. NQR spectra of molecular compounds.

Mossbauer Spectroscopy: Principles of Mossbauer spectroscopy, Doppler shift, Application of Mossbauer spectra for chemical structure determination, Numerical problems.

Suggested reading:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. P. W. Atkins & J. de Paula, Physical Chemistry (8th edn.), OUP (2006). Oxford University Press.
3. K. Zeemanski, *Thermodynamics.*
4. N.K.Adams, *Physics and Chemistry of Surface,*
5. A.W.Adamson, *Physical Chemistry of Surface,*
6. M.J.Rosen, *Surfactants and Interfacial Phenomena*, (1978) John Willey, New York.
7. Y.Moroi, *Micelles: Theatrical and Application Aspects*, (1992) Plenum Press, New York
8. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th edn., Tata McGraw-Hill, New Delhi (2002).
9. D. A. McQuarrie and J.D. Simon, *Physical Chemistry*, VIVA Students Ed. (2003)
10. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill International Edition

LABORATORY COURSE - II

PAPER: CHEM 804C (Organic Chemistry)

Total Marks: 150 (Theory 105 + Internal Assessment 45)

Credit: 06

1. Separation, purification and identification of compounds of binary solid mixtures by systematic qualitative analysis using different separation techniques like chromatographic techniques, steam distillation, fractional crystallization and sublimation
2. Identification of organic liquid compounds by distillation followed by systematic qualitative analysis
3. Organic preparation involving rearrangement reaction, condensation, nucleophilic substitution, heterocycles synthesis and multicomponent reactions.
4. Organic estimation - Estimation of glucose, glycine, formic acid and acetic acid in vinegar.

Suggested Text and reference books:

1. Practical Organic Chemistry, A. I. Vogel, ELBS, 2002.
2. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern, 1980.
3. Comprehensive Practical Organic Chemistry: Qualitative Analysis, V. K. Ahluwalia and S. Dhingra, Universities Press (India) Ltd, 2000.
4. N. K. Visnoi, Advanced organic Chemistry practical
5. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
6. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).

Electives

PAPER: CHEM 805E (Bio-inorganic Chemistry)

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credit: 02

Unit I: 5L

Calcium in Biology: Biochemical role of calcium, Storage and transport of calcium, Role of Ca^{2+} in muscle contraction, Blood clotting mechanism, Biological calcification.

Unit II: **5L**

Metallo-proteins and Metallo-enzymes of Fe : Ferritin, Transferrin, bio–mineralization and Siderophores, Peroxidase, Catalase, Hemerythrin, Cytochromes, Cytochrome P-450, Iron sulphur proteins, Rubredoxins, Ferredoxins.

Unit III: 5L

Metallo-enzymes and proteins of copper and zinc : Blue-copper proteins, Ceruloplasmin, Hemocyanin, Cytochrome-c oxidase, Superoxide dismutase, Carbonic anhydrase, Alcohol dehydrogenase, Carboxy peptidase, Metallothionein, inter changeability of Zn and Co in enzymes.

Unit IV: 9L

Biochemical role of Co, Mo and Mn : Biological nitrogen fixation, Vitamin B_{12}, B_{12}coenzyme, Cobalamines, Xanthine oxidase, Sulphite oxidase, Nitrite reductase, Arginase, Mn-SOD, Chlorophyll, Photosystem I and II, cleavage of water.

Metals in medicines: Toxicity of Hg, Cd, Pb, Cr, Be, Se, and As. Biological defence mechanism, Chelation therapy, Metals in diagnosis and Chemotherapy, Pt- complexes as anticancer drugs, Metal complexes as drugs.

Suggested Reading:

1. Bioinorganic Chemistry, Asim K. Das. Books & Allied Ltd, 2013
2. Bioinorganic Chemistry (Bertini, Ivano G, Harry B ,Lippard, S. J, Valentine, J.S.), University Science Books, CA, 1994.
3. J.A. Cowan, Inorganic Biochemistry: An Introduction, 2nd Edition, Wiley-VCH , 1997
4. R. P. Hanzlik, Inorganic Aspects of Biological and Organic Chemistry,, Academic Press, New York, 1976

PAPER – CHEM 806E (Bio-organic Chemistry)
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: **6L**

Chemistry of amino acids and peptides: Introduction to amino acids, nomenclature of α-amino acids; structures, properties and synthesis of natural peptides and peptide synthesis, different strategies in peptide synthesis, solid phase methods; sequencing of polypeptides; preliminary concept of protein and their structures; protein denaturation; biosynthesis of amino acids.

Unit II: **6L**

Structure and function of sugar derivatives -deoxy, amino, branched chain sugars; Disaccharides (sucrose, maltose, lactose); carbohydrate metabolism; role of sugars in biological recognition. Polysaccharides of biological importance, dextran, sialic acid and cyclodextrin

Unit III: **6L**

Classification of lipids, biological importance of fatty acids and lipids, essential fatty acids: ω-3and ω-6 fatty acids; Oxidation of fatty acids (alpha, beta, and omega), ketone bodies, fatty acid metabolism; Structure, sources and functions of prostaglandins, biosynthesis of prostaglandins, inhibition of prostaglandin synthesis; Synthesis of prostaglandins (PGE_2, PGE_3 PGF_2 and PGF_3).

Unit –IV: **6L**

Structure, functions and stability of some macrocyclic compounds, synthesis and different strategies adopted in the synthesis of exaltone, civetone and muscone.

Suggested Readings:

1. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford.
2. G. C. Barrett and D. T. Elmore, Amino acids and peptides (2004), Cambridge University press.
3. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
4. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
5. Chemistry of Biomolecules : An Introduction, R. J. Simmonds, RSC, 1992.
6. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7th Edition. W H Freeman & Co (Sd). 2017.
7. Biochemistry, C.B. Power and G.R. Chatwal. Himalayan Publishing House. 4th edition 1999.
8. J.E Vance, D.E Vance, Biochemistry of Lipids, Lipoproteins and Membranes. Amsterdam: Elsevier (2002).

PAPER - CHEM 807E (Surface Chemistry)
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit –I: Adsorption isotherm: **12 L**

Thermodynamics of adsorption isotherm, Different adsorption isotherms, Adsorption at solid-liquid, liquid-gas, liquid-liquid interfaces, Effect of added electrolyte on the surface excess of ionic surfactants.

Mixed surfactants: Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, counter ion binding in mixed surfactants.

Unit –II: Solubilisation and emulsification: **12 L**

Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions and applications.

Reference Books:

1. N.K.Adams, *Physics and Chemistry of Surface,*
2. A.W.Adamson, *Physical Chemistry of surface,*
3. M.J.Rosen, *Surfactants and Interfacial Phenomena*, (1978) John Willey, New York.
4. Y.Moroi, *Micelles: Theatrical and Application Aspects*, (1992) Plenum Press, New York

PAPER – CHEM 808E
Quantum Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit -I: Quantum Chemistry-I **12 L**

Interpretation of wave function (probability density).Box normalization.Superposition principle and expansion theorem. Derivation of the expression of L_z in polar coordinate system.P_x, L_z and $\hat{H}$ operators are Hermitian: Proof. Unitary and projection operators.Some important theorems. Schmidt orthogonalization.Dynamical variables and operators, dynamical states.Expectation value and average value. Linear vector spaces in quantum mechanics. Completeness theorem.Equations of motion of classical mechanics (in brief).Poisson bracket and Dirac's version of Correspondence principle. Ehrenfest theorem.Constants of motion.

The Heisenberg Uncertainty relations (position and momentum, angle and angular momentum , time and energy relations) : proof. Commutability and compatibility. Complete set of commuting operators. Fourier transform. Wave packet. Momentum space wave function.

Angular momentum operators (single particle system). Step up and step down operators. Spin angular momentum operators. Angular momentum operators (many electron system) and their commutation with spin free Hamiltonian operator. coupling of angular momenta, L-S coupling and j-j coupling. Term symbols and spectroscopic states. Pauli spin matrices and anti-commutation relations.

Unit -II : Quantum Chemistry-II **12 L**

Time independent non-degenerate perturbation theory (RSPT). Application: ground state of He atom. Degenerate RSPT. Applications: Stark effect, normal and anomalous Zeeman effect. Rayleigh- Ritz variation principle.Linear variation method. Applications: ground state energy of Heatom, harmonic oscillator.

Time dependent RSPT (First order).Fermi-Golden rule. Born-Oppenheimer approximation(in detail). Antisymmetrized wave Function. Slater determinant and Pauli exclusion principle.

Reference Books:

1. L.I. Schiff, *Quantum Mechanics*, Third Edition, McGRAW-HILL BOOK COMPANY, 1985.
2. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford UniversityPress.
3. B.H. Bransden& C.J. Joachain, *Physics of Atoms and Molecules*, Longmann Scientific and Technical, 1994.
4. B.H. Bransden& C.J. Joachain, *Quantum Mechanics*, Second edition, low price edition, PEARSON Education, First Indian Reprint, 2004.
5. J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesely Publishing Company.
6. Eugene Merzbacher, *Quantum Mechanics*,Wiley International Edition, 1970.

SEMESTER III

INORGANIC CHEMISTRY - III
PAPER - CHEM 901C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credits: 04

Unit: I Reaction Mechanism of Transition Metal Complexes 12L

Stepwise and overall formation constants, Factors affecting the stability of metal complexes, chelate effect, determination of binary formation constants, Energy profile of reactions, Labile and inert complexes; dissociative, associative and interchange mechanisms of ligand substitution reactions, mechanisms of ligand-replacement reactions, ligand substitution reactions in square planar and octahedral complexes, mechanisms of ligand-replacement reactions trans effect, acid & base hydrolysis; ; isomerisation and racemisation of tris-chelate complexes, Ray-Dutta and Bailar twist mechanisms. Mechanism of electron transfer (redox) reactions: inner and outer sphere reactions, complementary and non-complementary reactions, stereochemical non-rigidity and fluxional molecules

Unit II π-Acid complexes and Clusters 12L

Transition metal π-acid complexes: π-acid ligands (CO, NO, tertiary phosphine, arsine), structure, bonding, synthesis and reactivity of complexes of CO, NO, tertiary phosphine, metal carbonyl hydrides.

Metal carbonyls, clusters and Metal-metal multiple bond:

Metal clusters: Low nuclearity and high nuclearity carbonyl clusters; Boron clusters: Structure and bonding of boranes and Lipscomb's topology, styx system of numbering, nomenclature; Synthesis and structure of carboranes, metalloboranes, metallocarboranes; Skeletal electron counting, Wade's rule. Metal-metal multiple bond, quadruple bond, structures and bonding (MO).

Unit III: X-ray crystallography **12L**

Crystals Lattices and symmetry: Lattice points, Unit Cells, ; Symmetry operations and elements of symmetry, Point groups, Classification of unit cells, Crystal systems, Herman-Mauguin notation, Bravais Lattices, Distinction between trigonal and hexagonal systems, Crystal planes and indices Law of rational indices.

Space groups and equivalent positions: Screw axis, Glide planes, Space groups, Relationship between space groups, point groups, Equivalent positions, Special positions,

X-ray diffraction : and Bragg's law; Crystal systems and symmetry, point groups, stereographic projection of 32 point groups and space groups-Hermann–Mauguin notations,; Primitive and non-primitive unit cells; Symmetry elements: isogonal symmetry groups and reciprocal lattice.; X-ray-instrumentation Data collection, data reduction, refinement and structure solution

Unit IV Transition metal chemistry: **12L**

Inner transition Metals : comparative study of Lanthanides and Actinides with reference to oxidation states, complex formation, magnetic properties, colour and spectral properties, Lanthanide shift reagents.

Platinum Metals:

General discussions: position in periodic Table, electronic configurations, oxidation states, general trends in properties, Important compounds of Ruthenium, Rhodium, Iridium, osmium, palladium and platinum- synthesis, structure , properties and applications...

Suggested Readings:

1. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5th Edition, Wiley Interscience, N.Y
2. J. Huhee, E.A. Keiter, R.L. Keiter& O.K. Medhi-Inorganic Chemistry-Principles of Structure and Reactivity, 5thEdn..Pearson Education, 2007.
3. Crystal Structure Determination, William Clegg, Oxford University Press, 1998.
4. Structure Determination by X-ray Crystallography, Mark Ladd and Rex Palmer (September 30, 2003).
5. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
6. Shriver & Atkins - Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
7. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984).
8. F. Basolo & R. G. Pearson, Mechanism of Inorganic Reactions, Wiley Eastern (1967)

ORGANIC CHEMISTRY – III
PAPER - CHEM 902C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credits: 04

Unit I: Nuclear magnetic resonance spectroscopy for organic compounds 16L

Relaxation phenomenon in NMR, broadening of signals, sample handling and solvent for NMR study, chemical shift, internal standards, factors affecting the chemical shift, spin-spin coupling, multiplicity of splitting and relative intensity of lines, coupling constant, first order and non-first order splitting, vicinal and geminal coupling, long range coupling – two bond coupling (2J) three bond coupling (3J), Nuclear overhauser effect (NOE), Karplus relationship. Designation of spin systems. Chemically induced dynamic nuclear polarization (CIDNP). Interpretation of PMR spectra. **^{13}C NMR spectroscopy:** Principle, multiplicity, proton –decoupling, off-resonance decoupling, noise-decoupling, ^{13}C chemical shifts values, DEPT and INEPT terminology; Two dimensional NMR spectroscopy: magnetic resonance imaging (MRI). Applications of NMR in the structure elucidation of organic compounds.

Unit II: Mass spectroscopy for organic compounds 8L

Introduction – basic theory, instrumentation and sample handling. Methods of generation of mass ions – electron impact (EI), chemical ionization (CI), electron spray ionization (ESI) and fast atom bombardment (FAB) techniques, TOF-MALDI and SELDI; Tandem mass spectroscopy, general mass fragmentation pattern of organic compounds, base peak, molecular ion, relative intensity, mass ions fragmentation, metastable ions, even electron rule, nitrogen rule, HDI, application of mass spectroscopy.

Unit III: Main group Organometallic Chemistry: 12L

Introduction, importance of organometallic compounds as reagents, additive and catalyst. Chemistry of organolithium, magnesium, zinc, copper, aluminium, cadmium and mercury - synthesis, structures and reactivity. Stability, preparation and reactivity of metal alkyls, aryls and hydrides.Applications of main group organometallics in organic synthesis.

Unit IV: Transition metal based Organometallics in organic synthesis 12L

General- Ligands, bonding, haptonumber, stability, synthesis and reactivity. Uses of Organo-transition metal reagents of chromium, cobalt, iron, nickel, rhodium and palladium in organic synthesis; sandwich compounds and their reactivity, Tebbe reagent.

Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene metal group complexes, η6-arene-chromium tricarbonyl in organic synthesis

Palladium catalyzed C–C coupling reactions: The Heek reaction, Suzuki-Miyaura coupling, Sonogashira coupling, Stille coupling, Kumada coupling, Negishi coupling.

Suggested readings:

1. High-Resolution NMR Techniques in Organic Chemistry, Third Edition, 2016, by Timothy D.W. Claridge, Oxford, United Kingdom. Published by Elsevier Ltd.
2. Organic Spectroscopy- Principles and Applications, Jag Mohan, Narosa publishing House.
3. Spectroscopic Methods in Organic Chemistry, By D.H. Williams, I. Fleming. Tata McGraw Hill Pub. Co. Ltd.
4. Organic Spectroscopy, 3rd Edn, By William Kemp. Published by Palgrave, NewYork.

5. The Organometallic Chemistry of The Transition Metals. By Robert H. Crabtree, Yale University, New Haven, Connecticut. Published By John Wiley & Sons, Inc., Hoboken, New Jersey. Isbn 0-471-66256-9.
6. Organometallics in Synthesis - A Manual. Edited by Manfred Schlosser. Published by John Wiley & Sons Ltd.
7. Handbook of Functionalized Organometallics - Applications in Synthesis. Volume -1 By Paul Knochel. Published by Wiley-VCH Verlag GmbH & Co.
8. Metallo-Organic Chemistry. By A.J. Pearson. John – Wiley & Sons.
9. Organotransition Metal Chemistry : Applications to organic synthesis, Stephen G Davies Pergman Press
10. Organolithiums: Selectivity for synthesis, Jonathan Clayden, Pergamon, 2002
11. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press.

PHYSICAL CHEMISTRY - III
PAPER – CHEM 903C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 04

Unit -I: Polymer Chemistry 12 L

Polymer and Characterisation:-Banz concepts of polymer science, Molecular forces and chemical bonding in polymers.Polymer solution and fractionation. Gel permeation Chromatography and molecular weight determination by viscometry, osmometry, light scattering and ultra centrifugation, molecular weight distribution curve.

Polymerization:- mechanism and kinetics of step growth and chain growth polymerization- radical, ionic and ring opening polymerization, copolymerization, polymerization techniques and polymer reaction, polymer structure and physical properties: configuration of polymer chain crystal structure of polymers: speciality polymers: Block copolymer, polymer colloids and biomedical polymers.

Unit -II: Chemical Kinetics-II: 12 L

Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple; Bi-molecular reactions; Collision theory; Activated complex theory.Reactions in solutions: Diffusion controlled and activation controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength; Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed uni-molecular and bimolecular reactions; Applications in ammonia synthesis and oxidation of carbon-monoxide.

Unit -III: Electrochemistry-I: 12 L

Activity in electrolytic solutions.Freezing point depression and the mean ionic activity coefficient.The Debye-Huckel theory for dilute ionic solutions (derivation) and correction for concentrated solutions Equilibrium in ionic solutions.Ion association.

Unit -IV: Solid State Chemistry: 12 L

Review of the basic concepts: Bragg's law, Miller indices, Elements of symmetry (plane, axis and centre of symmetry). X-ray diffraction: powder method, principle and applications.

Crystal Defects: Point defects, Stoichiometric and non-stoichiometric defects, Kroger-Vink notation for crystal defects, thermodynamics of Schottky and Frenkel defect formation. Metals, insulators and semiconductors; intrinsic and extrinsic semiconductors, p-n junction.

Solid Solutions: Substitutional, interstitial and subtractional solid solutions & distortions

Reference Books:

1. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
2. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
3. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
4. G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
5. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
6. F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New York.
7. K.J.Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
8. H. Eyring, S. H. Lin and S. M. Lin, *Chemical Kinetics* (1999), Jhon Willey, New York.
9. J.O'M, Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Vol.1&2 (1998), Plenum Press, New York.
10. A. R. West *Solid State Chemistry and its Applications*, John Wiley (2001).
11. Crystal Structure Analysis, Jenny Glusker and Kenneth Trueblood (August 1992).
12. N. B. Hannay. *Solid State Chemistry*, Prentice-Hall (1979).
13. D. K. Chakraborty. *Solid State*, New Age International, New Deldi (1996)

LABORATORY COURSE-III

Paper: CHEM 904C (Physical Chemistry)

Total Marks: 150 (Practical 105 + Internal Assessment 45)

Credit: 06

Laboratory Course in Physical Chemistry

1. Determination of specific rotation of cane sugar and determination of concentration of supplied sample.(Quantitative-one day).
2. Potentiometric titration of Co(II) by $K_3[Fe(CN)_6]$and determination of concentration of Co(II) in a solution. (Quantitative-one day).
3. Conductomectric titration of triple mixture containing KCl, NH_4Cl and HCl by $AgNO_3$ and by NaOH solution. (Quantitative-one day).
4. Verification of Beer's law and determination of concentration of unknown solution spectrophotmetrically(Quantitative-one day).
5. Determination of strengths of halides in a mixure ,potentiometrically.
6. Determination of pH of buffer solutions and hence to calculate the E^0 of quinhydrone electrode
7. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
8. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.
9. Determination of rate constant and order of the reaction between $KBrO_3$ and KI in acid medium.(Qualitative- one day)
10. Kinetic study of decomposition of $K_2S_2O_8$ by KI and effect of added salt. (Qualitative- two day)
11. Determinaton of formula of cupro-ammonium ion. (Qualitative- one day)
12. Determination of standard electrode potential of quinhydrone electrode. (Qualitative-one day).

13. Determination of composition and stability constant of Ferric-salicylic acid complex by Job's method. (Qualitative-two day).
14. Determination of critical micellarconcentration(CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.

Reference Books:

1. D. P. Shoemaker, C. W. Garland & J. W. Nibler. *Experiments in Physical Chemistry* (5^{th}edn.), McGraw Hill (1989)
2. Findlay's Practical Physical Chemistry, 9^{th} Ed. Revised by B.P. Levitt, Longman.1973.
3. V. D. Athawala& P. Mathur. *Experimental Physical Chemistry*, New Age InternationalPublishers (2001).

ELECTIVES

PAPER - CHEM 905 E
Special Topics in Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit-I: SUPRAMOLECULAR CHEMISTRY 12L

Concepts and Languages of supramolecular chemistry - Molecules, super molecules; factors leading to strong binding (non-covalent interactions); molecular receptors – design and principles; Types of supramolecular interactions (Hydrogen bonding, vander Waal's interaction, π-stacking, CH-π, anion-π interaction). Supramolecular chemistry in inorganic perspective: Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Types of interactions between host and guest molecules;Thermodynamics of host-guest complexation; Enthalpy and entropy contributions, complexation free energies; Molecular recognition – factors involved; Molecular receptors – for alkali metal ions, ammonium ions, anions and neutral molecules. Crownethers, cryptands, spherands and ionophores; Creation of rotaxanes, catenanes and cyclophanes; Supramolecular catalysis- Catalysis by Reactive Macrocyclic Cation Receptor Molecules; Application of supramolecular chemistry in catalysis, drug delivery, recognition/sensing and material science.

Unit –II: NANO CHEMISTRY 12L

Background to Nano-science and Technology - Implications for Physics, Chemistry, Biology and Engineering - Classifications of nanostructured materials - nano particles - quantum dots, Nanowires, nano-tubes – ultra – thinfilms – multilayered materials; Typical syntheses of nano particles, oxide nano tubes and fibres, metal nano particles; Length Scales involved and effect on properties: Mechanical, Electronic, Optical, Magnetic and Thermal properties.

Synthesis of nanoparticle: Bottom-up Synthesis -Top-down Approach: Precipitation, Mechanical Milling, Colloidal routes, Self-assembly, Vapour phase deposition, MOCVD, Sputtering, Evaporation, Molecular Beam Epitaxy, Atomic Layer Epitaxy, MOMBE.

Characterization of nano particles- X-ray diffraction technique, Scanning Electron Microscopy - environmental techniques, Transmission Electron Microscopy including high-resolution imaging, Surface Analysis techniques

Application of nano-structured material in organic synthesis, dendrimers, bucky balls and nano tubes (properties and applications), drug delivery systems; Nanotechnology for sustainability, Nanomedicine, Environmental, health, and safety issues

Suggested reading:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. A.S. Edelstein and R.C. Cammearata, eds., Nanomaterials: Synthesis, Properties and Applications, (Institute of Physics Publishing, Bristol and Philadelphia, 1996)
3. N John Dinardo, Nanoscale charecterisation of surfaces & Interfaces, Second edition, Weinheim Cambridge, Wiley-VCH, 2000
4. G Timp (Editor), Nanotechnology, AIP press/Springer, 1999
5. AkhleshLakhtakia (Editor) The Hand Book of Nano Technology, "Nanometer Structure", Theory, Modeling and Simulations. Prentice-Hall of India (P) Ltd, New Delhi, 2007.
6. Desiraju, G. R. Crystal Design: Structure and Function, (John Wiley & Sons, 2003).
7. Steed, J. W.; Atwood, J. L. Supramolecular Chemistry, (John Wiley & Sons, 2009).

PAPER: CHEM 906E

Chemistry of Natural products

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT - I **6L**

General: Sources and types of natural products, method of isolation and structure elucidation, importance of natural products, biosynthesis of some common type of natural products *viz.* terpeneoids, steroids, flavonoids and alkaloids.

UNIT- II **6L**

Chemistry of terpenoids: General methods of determining structure, correlations of configurations, sesquiterpenoids, diterpenoids, triterpenoids with special reference to the isolation, structure and stereochemistry. Chemistry of Caryophyllene and isocaryophyllene, abietic acid and Gibberellic acid.

UNIT- II **6L**

Alkaloids and Phenolics - Chemistry of quinoline, isoquinoline, phenanthrene and indole group of alkaloids - papaverine, cimchonine quinine, morphine, thebaine, codeine, reserpine with special reference to isolation, structure and stereochemistry. Plant phenolics with special reference to the general structures, reactions and synthesis of anthocyanins, anthocyanidins, flavones flavonols, isoflavones, chalcones, coumarins, quinines and tannins.

UNIT IV **6L**

Steroids and hormones: Classification and nomenclature of steroids, Structure, spectral properties of steroids, stereochemistry of steroids, reaction of steroids, chemistry of cholesterol, ergosterol, vitamin D, bile acids, steroid hormones- oestrone, progesterone, testosterone., artificial hormones, Miscellaneous transformations of steroid molecules- steroidal glycosides and alkaloids.

Reference books:

1. Organic Chemistry, I.L. Finar, volume 2, ELBS, 5th edition (1975).
2. Organic Chemistry. Morrison Boyd and Bhattacharjee, 7th edition (2013), Pearson.
3. Chemistry of Plant Natural Products - Stereochemistry, Conformation, Synthesis, Biology, and medicine. Vol 1 and Vol 2. Springer Heidelberg New York Dordrecht London. 2015

PAPER: CHEM 907E
Environmental and Green Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit – I: Environmental Chemistry 12L

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, Ozone depletion, The green-house effect and Global warming, El-Nino phenomenon. Micro-organism in aquatic chemical reactions, Eutrophication, Re-cycle of waste-water in process industry, Treatment of sewage and reuse of water in industry and agriculture, microbiologically mediated redox reactions and Nitrogen transformation by bacteria. Water pollutants: Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity, DO, BOD, COD etc.); industrial and waste-water treatment; Chemical hazards, chemical disaters, pollution of environment-man made, industrial, natural disasters, environmental biochemistry, toxicological chemistry; analysis of water and waste water, solid wastes and air pollution-Photochemical smog, Auto exhausts, Acid-rains, Air-quality standards. Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

Unit – II: Green Chemistry 12L

Definition, Concepts and basic principles of green chemistry, need of green chemistry, green chemistry as an alternative tool for reducing pollution, atom economy, less hazardous chemical syntheses, atom economy in rearrangements, addition and pericyclic reactions, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, Green synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology. Development of new methods for organic synthesis such as Green Synthesis: use of sonochemistry, use of ionic liquids, use of microwaves, bio-catalysis. Selection of solvent: i) Aqueous phase reactions ii) Reactions in ionic liquids iii) Solid supported synthesis iv) Solvent free reactions, Green catalysts: i) Phase transfer catalysts (PTC) and ii) Biocatalysts. Microwave and Ultrasound assisted green synthesis: Aldol condensation, Cannizzaro reaction, Diels-Alder reactions, Strecker synthesis, Willaimson synthesis and Dieckmann condensation.

Book Suggested:

1. Handbook of Environmental chemistry, Springer-Verlag, O. Hutzinger.
2. M. Bernhard, F.E. Brinckman & P.J. Sadler.The Importance of Chemical Speciation in Environmental Processes, Springer-Verlag,
3. L.J. Fristschen, & L.W. Gay, Environmental Instrumentation, Springer-Verlag,.
4. Real World Cases in Green Chemistry, ACS, M.C. Cann & M.E. Connelly.
5. P.T. Enastas and T.C. Williamson, Green Chemistry: Designing Chemistry for Environment, ACS,
6. Green separation processes, methods and application, Fonso, National Scientific Book Agency, Delhi-110053.

7. G.W. Vanloon, S.J. Duffer, Environmental Chemistry - A Global Perspective, (2000) Oxford University Press.
8. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.
9. Colin Baird, Environmental Chemistry, (1995) W.H. Freeman and Company, New York.
10. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
11. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.
12. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
13. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India,New Delhi

PAPER - CHEM 908 E
Advanced Group Theory
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit -I: Group Theory – I: 12 L

The concept of groups; group multiplication tables and the rearrangement theorem; subgroups, classes and the related theorems; commutative groups (Abelian), cyclic group; isomorphism and homomorphism. Examples.

Molecular point groups (in Brief) , similarity transformation and the invariance of characters of matrices under such transformation, matrix representation of point groups; reducible, irreducible and equivalent and inequivalent representations; the great orthogonality theorem (no derivation) and its corollaries, character tables, construction of character tables in complex cases such as $D_{6h,}$ $T_d$etc; the group of Schrodinger equation; basis function for irreducible representation "projection" operator; direct product representation .

Unit -II: Group Theory - II (Physical Applications): 12 L

Symmetry factoring of secular equations; LCAO -MO ,II bonding and Huckel's theory ;some examples: ethylene ,bengene ,Naphthalein. symmetry based "selection rules" for cyclization reaction (Woodward Hoffmannrule) Hybrid orbital and Molecular orbitals for AB_n -type molecules. Crystal field theory (CFT) Splitting of energy levels, and terms in a chemical environment. Determining the symmetry types of the normal modes;selection rule for fundamental (infra-red and Raman) vibrational transitions. Mutual Exclusion rule.

Reference Books:

1. Chemical Application of Group Theory – F.A. Cotton,3rd edition, A Wiley Interscience publication
2. Group Theory and Quantum Mechanics, M.Tinkham, Tata McGraw Hill, publishing Ltd.
3. Group Theory and Chemistry, David M. Bishop, Clarendon Press Oxford.
4. Group Theory and its application to Physical Problem, M. Hamermeah, Dover publication.

SEMESTER IV

INORGANIC CHEMISTRY-IV
PAPER: CHEM 1001C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credits: 04

UNIT I - Basic Organometallic Chemistry: 12L

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, Ligands in organometallic chemistry; Synthesis, bonding and reactivity of Metal-alkyl, -alkene, -alkyne, -allyl, -carbene, -carbyne and -carbide complexes, Agostic interaction, Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples; Chemistry of η3 -η6 cyclic,sandwich and half-sandwich transition metal complexes. Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene -metal complexes.

UNIT II - Catalysis Using Organometallic Compounds: **16L**

Terminology in catalysis (Turnover, Turnover number, Turnover frequency or turnover rate, mole fraction, eantioselectivity, stereoselectivity, chemoselectivity, regioselectivity); Catalytic Hydrogenation of alkenes and related reactions: Hydrogenation catalysts, Catalytic cycle of Wilkinson's catalyst, Catalytic asymmetric synthesis, the mechanism of asymmetric hydrogenation using a chiral catalyst.

Olefin Metathesis: synthesis of Grubbs' and Schrock catalysts, Mechanism of olefin metathesis, ring opening metathesis, cross metathesis, ring closing metathesis, ring opening polymerization metathesis, acyclic diene metathesis polymerization, enyne metathesis

Olefin polymerization and oligomerisation reactions: The Ziegler-Natta catalyst, site control and chain end control mechanisms, metallocene based catalysts, post metallocenes catalyst.

UNIT III Inorganic polymers: **8L**

Classification of inorganic polymer, inorganic polymerisation reactions (addition,condensation and coordination polymerisation). Polysiloxanes, polysilanes, poly phosphazenes, polymeric sulfur;

Coordination Polymers: Definition, classification and design strategies, network topologies, supramolecular isomerism, interpenetration, porous coordination polymers, properties and applications

Unit IVInorganic Photochemistry 12L

Introduction to inorganic photochemistry, photophysical and photochemical process, characteristics of the electronically excited states of inorganic compounds, ligand field states, charge transfer states; Photochemical processes: Selection rules, Jablonski diagram, Fluorescence and phosphorescence, delayed fluorescence, Photochromism, Photosensitization, Quantum yield; Photochemical reactions: substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes; Application of inorganic photochemistry: Molecular recognition, Sensing, Photochemical splitting of water, Dye sensitized solar cells.

Suggested Reading:

1. Organometallic Chemistry- A Unified Approach, R. C. Mehrotra. And A.Singh,New Age International , Ltd. New, Delhi.

2. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5th Edition, Wiley Interscience, NewYork.
3. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984.
4. Shriver & Atkins - Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
5. Fundamentals of Photo chemistry, K.K.Rohatgi- Mukherjee, New Age International Publishers, New Delhi
6. A.W. Adamson & P.D. Fleischauer. Concepts of Inorganic Photochemistry, John Wiley & Sons (1975).

ORGANIC CHEMISTRY – IV
PAPER: CHEM 1002C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credits: 04

Unit I: Heterocyclic chemistry **12L**

Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; Basicity and aromaticity of heterocycles; Synthesis, properties and reactions (ring openings & heteroatom extrusion) of 3- membered heterocycles (aziridines, oxiranes and thiiranes), 4- membered heterocycles (azetidine, oxetanes and thietanes); Synthesis and reactivity of azoles (imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiazole and their benzo derivatives) and azines (6-membered heterocycles with two hetero atoms -pyridazines, pyrimidines and pyrazines), caffeine; theobromine and theophylline.

Unit II: Nucleic acids and enzymes **12L**

Introduction, nucleic acid bases, Purine and pyrimidine bases of nucleic acids, nucleosides and nucleotides, their structures and nomenclature, structures and functions of NADH, NADP and ATP, Structures of RNA and DNA; DNA base-pairing, double helical structure of DNA, replication of DNA and mutagenesis, codon, anticodon, t-RNA, structure and genetic code, transcription and translation

Enzymes: nomenclature, stereochemical aspects, Mechanism of enzyme action, kinds of reactions catalyzed by enzymes, cofactors, co-enzyme chemistry. **Application and enzyme catalytic organic reactions** – Oxidation, reduction, isomerization, epimerization, hydrolysis, phosphorylation, acylation, methylation, decarboxylation, dehydration. Enzymatic hydrolysis of peptides (carboxy peptidase, trypsin, chrymotrypsin and Lys C);

Unit III- Drugs and drug design: **14L**

Concepts of drugs, classification, analogues and pro-drugs, theories of drug action, assay and metabolism of drugs; Drug design, theory of drug design, structure activity relationship (SAR), Quantitative structure activity relationship (QSAR); prodrugs and soft drugs; ADME.

Synthesis and uses of the following drugs of different pharmacological activities:

a) Antimalerials: Quinine, chloquine, Trimethoprim
b) Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.
c) Anti-inflammatory:Aspirin, Ibuprofen, Diclophenac, Indomethacin, coxib
d) Antitubercular and antileprotic: Ethambutol, Isoniazide&Dapsone

e) Anaesthetics: Lidocaine, Thiopental.
f) Antihistamines: Phenobarbital, Diphenylhydramine.
g) Tranquilizers: Diazepam, Trimeprazine
h) Cardiovascular: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol

Unit IV: Chromatography and optical microscopy: 10L

Basic concept of chromatographic separation – adsorption and partition chromatography, theory and handling of different chromatographic techniques – thin-layer, column, and paper chromatography; Gas chromatography: Basic principle, basic instrumentation, column types and column selection; detectors (FID, TCD, ECD, NPD); sample separation and applications. High performance liquid chromatography (HPLC): Instrumentation - basic equipment; pumping and injection system, column and its packing materials, normal and reverse phases; detectors, sample separation and application. Gel permeable (filtration) chromatography, Size exclusion chromatography, Gel electrophoresis.

Optical microscopy: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.

Recommended text and reference books:

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Pearson Education
5. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7th Edition. W H Freeman & Co (Sd). 2017.
6. Bioorganic and Bioinorganic and Supramilecular Chemistry. P.S. Kalsi, New Age International (Pvt. Ltd.) 2nd edition 2010.
7. A. Kar, Medicinal Chemistry, New Age publication
8. Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-A Molecular and Biochemical Approach, Oxford University Press.
9. Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
10. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-HilI (2005).
11. S. S. Pandeya& J. R. Dimmock.Introduction to Drug Design, New Age International.(2000).
12. D. Lednicer. Strategies for Organic Drug Synthesis and Design, John Wiley (1998).
13. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).
14. Principles and Practice of Modern Chromatographic Methods, (1st Edition), Robards, Jackson & Haddad, Academic press (1994).
15. Chromatographic Methods (5th Edn), A. Braithwaite, J.F. Smith, Kluwar Academic Publisher.

PHYSICAL CHEMISTRY - IV

PAPER – CHEM 1003C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

Unit - I. Statistical Thermodynamics 12 L

Independent subsystems and distinguishability.Boltzmann distribution (nondegenerate and degenerate cases). Review of partition function: Thermal De Broglie wavelength. Partition functions for electronic, nuclear, rotational and vibrational degrees of freedom. Thermodynamic quantities in terms of partition functions.Entropy of ideal gas.Gibbs paradox. Equilibrium constants (ideal gas reaction) in terms of partition function.

The mathematical proof of the equipartition of energy principle.Specific heats of solids, fluctuations.

Unit - II : Photochemistry 12 L

Physical properties of excited molecules:

Nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids. Polarisedluminencence, non radiative intra-molecular electronic transition, internal conversion, intersystem crossing, crossing potential energy surface (Franck- Condon factor).

Photo-physical processes in excited state:

Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation. Mechanism of quenching, energy transfer process (Forster dipole coupling), electron transfer phenomenon (Marcus theorem, Rehm Weller theorem), eximer. Laser

Unit -III: Bio-physical Chemistry: 12 L

Hydrophobic effect and self organising systems, structure and functions of proteins and nucleic acids and their stability.Structure and functions of cell membranes; Ion transport through cell membranes and nerve conduction; Multiple equilibria; stacking and cooperative interactions in biological systems. Muscle contraction; Techniques for study of structure and functions of proteins and nucleic acids.

Unit -IV: Electrochemistry–II: 12 L

Electrodics - The basic electrodic equation: Butler-Volmer equation, overpotential, polarisable and non-polarizable interfaces;Faradaic and non -faradaic Currents, Over-potentials,aspects of deviation from equilibrium. Electrical conductance of solutions; The Debye HuckelOnsagarequation for conductance (derivation); Conductance at high fields and high frequencies, Conductance in non-aqueous solvents. Fuel Cells: H_2-O_2 cell, Air-H cell; Electricity producing cells: Na-S, Sb-S.

Numerical problems.

Reference books:

1. D. A.McQuarrie, *Statistical Mechanics,* (2003), Viva Books Pvt. Ltd. New Delhi.
2. M. C.Gupta, *The Statistical Thermodynamics*,(1990), New Age International (P) Ltd. New Delhi.
3. M.Dole, Introduction to Statistical Thermodynamics

4. K.K.Rohtagi-Mukherjee, *Fundamental of Photochemistry*,(1986) New Age International New Delhi.
5. J. G. Calvert and J. N. Pitts, Jr., *Photochemistry* (1966) John Wiley & Sons, New York.
6. R. P. Wayne, *Principles and Application of Photochemistry* (1988), Oxford University Press, Oxford.
7. N. J. Turro, *Modern Molecular Photochemistry*, (1991) Univ. Science Books, Sansalito.
8. J. F. L Lakowicz, *Principles of Fluorescence Spectroscopy*, 2nd Edn. (1999) Planum Publishers, New York.
9. L. Lehninger. *Biochemistry*, 8th edition, Kalyani Publishers (2008).
10. G. Thomas. *Medicinal Chemistry: An Introduction*, 2nd Edition, Wiley (2007).
11. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
12. A. R. West *Solid State Chemistry and its Applications*, John Wiley (2001).

CHEMISTRY PROJECT - I

PAPER: CHEM 1004C

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credit: 02

To be carried out under the guidance of an assigned faculty member of the Department. Area of research topics or any specific topic will be given to the student concern for preparation of literature report that to be submit for evaluation.

CHEMISTRY PROJECT - II

PAPER: CHEM 1005C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

To be carried out under the guidance of an assigned faculty member of the Department. **Project Report Submission and presentation (experimental / theoretical work)**