INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-501** Course Title: **Quantum Chemistry, Symmetry and Group Theory**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**
4. Relative Weight**: CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite: Nil
9. Objective: To provide basic concepts and mathematical treatment of atomic model, chemical bond, symmetry and group theory.
10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Quantum chemistry:** Basic postulates, eigenvalues and eigenvectors, Hermitian operators, applications including translational, vibrational and rotational degrees of freedom - particle in 1D/2D/3D box, particle in a ring, rigid rotor, harmonic oscillator. Electronic, vibrational and rotational transitions. Solution of Schrödinger equation for the hydrogen atom; radial and angular functions, atomic orbitals and electron spin. Multi-electron systems, term symbols.	**14**
2.	**Approximate techniques and chemical bonding:** Born-Oppenheimer approximation, variation and perturbation methods with examples. Valence bond theory including mathematical treatment of sp, sp^2 and sp^3 hybridized orbitals, molecular orbital theory with suitable examples, □uckel molecular orbital approach. Introduction to semi-empirical and *ab initio* methods.	**14**
3.	**Molecular symmetry and group theory:** The concept of groups, symmetry operations and symmetry elements in molecules, matrix representations of symmetry operations, point groups, representation of a group, reducible and irreducible representations, great orthogonality theorem and its consequences,	**8**
4.	**Applications of group theory:** Group theory and quantum mechanics, applications of group theory to atomic orbitals in ligand fields, molecular orbitals, symmetry of normal modes of vibrations, prediction of infrared, Raman active vibrational modes, and electronic transitions.	**6**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Levine, I. N. "Quantum Chemistry", 7th Ed., PHI Learning Pvt. Ltd., Delhi.	**2013**
2.	McQuarrie, D. A. "Quantum Chemistry" Reprint, Viva Books.	**2007**
3.	Atkins, P. "Molecular Quantum Mechanics", 4th Ed., Oxford University Press.	**2010**
4.	Cotton, F. A., "Chemical Applications of Group Theory", Reprint, Wiley Eastern.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-503** Course Title: **Thermodynamics, Interfaces and Solids**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**

4. Relative Weight**: CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**

8. Pre-requisite: Nil

9. Objective of Course: To familiarize the students with thermodynamics aspects of chemical phase equilibria, surface processes and ionic systems, and solids.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Classical thermodynamics:** Thermodynamic treatment of phase equilibria, thermodynamic properties of solutions, chemical potential, chemical potential of real gases and fugacity, thermodynamic function of mixing, thermodynamic treatment of ideal and non-ideal solutions, concept of activity, excess thermodynamic functions. Thermodynamic equilibria in one and two component systems.	**12**
2.	**Statistical thermodynamics:** Concept of microstates and ensembles, microcanonical, canonical and grand canonical ensemble, average distribution, partition functions and its relation with thermodynamics properties, Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac statistics, Molecular partition functions, translational, vibrational, and rotational partition functions. Ideal monoatomic and diatomic gases and their thermodynamic properties.	**10**
3.	**Thermodynamics of surfaces and interphases:** Surface and interfacial phenomenon, macromolecules, adsorption of gases by solids, BET theorem, determination of surface area of solids, adsorption from solution, electrical phenomenon of interphases.	**7**
4.	**Thermodynamics of ionic systems:** Thermodynamics of reversible and irreversible electrochemical systems, thermodynamic foundation of theory of ionic interaction and calculation of energy of ionic interaction, interpretation of electrical conductance of electrolytes, thermodynamic treatment of diffusion potential. Thermodynamics of different types of chemical processes accounting in living systems, metabolic and biosynthetic reaction, thermodynamics of ionic polymers.	**7**
5.	**Solids:** Structural classification of binary (AX, AX_2, etc.) and ternary (ABX, ABX_2, ABX_3, AB_2X_4, etc.) compositions, powder X-ray diffraction – Bragg's peak, absences, indexing of simple systems. Bonding in solids – introduction to metals, insulators and semiconductors, electronic structure of solids. Electrical conductivity, mobility, thermal conductivity, and specific heat of solids. Magnetic properties of solids, magnetization and susceptibility.	**6**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Seddon, J. M. and Gale, J. D., "Thermodynamics and Statistical Mechanics", Royal Society of Chemistry.	**2001**
2.	McQuarrie, D. A. and Simon, J. D., "Physical Chemistry", Reprint, Viva Student Edition.	**2013**
3.	McQuarrie, D. A., "Statistical Mechanics", Reprint, Viva Books Pvt. Ltd.	**2013**
4.	Atkins, P.W., "Physical Chemistry", 7th Ed., ELBS, Oxford University Press.	**2003**
5.	Silbey, R.J. and Alberty, R.A., "Physical Chemistry", 4th Ed., John Wiley & Sons, Inc., New York.	**2003**
6.	West, A. R., "Solid State Chemistry and its Applications" Reprint, Wiley, India	**1987**
7.	Wells, A. F., "Structural Inorganic Chemistry", 5th edn., *Clarendon Press, Oxford*	**1984**
8.	Spaldin, N. "Magnetic Materials: Fundamentals and Device Applications", *Cambridge University Press*	**2003**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject code: **CYN-505** Course Title: **Basic Analytical Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**
4. Relative Weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PCC**
8. Pre-requisite: Nil
9. Objective: To impart basic knowledge in different concepts of analytical chemistry.
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Measurement basics:** Signal and noise, sensitivity and detection, hardware and software techniques for enhancing signal to noise, accuracy and instrument calibration, basic electronic components and circuits for instrumentation used in chemical analysis, optical components for instrumentation used in chemical analysis.	**4**
2.	**Statistical concepts for analytical chemistry:** Error analysis, regression plots, criteria for rejection of data, Q-test, t-test, F - test, ANOVA, control chart, use of spreadsheet.	**6**
3.	**Spectral methods:** Spectrophotometry– Beer-Lambert law, its applications and limitations, single and double beam spectrophotometer, analysis of mixtures, fluorimetry, nephelometry, turbiditmetry. Atomic absorption spectrometry– principle and applications, flame emission spectrometry (flame photometry).	**7**
4.	**Electroanalytical methods:** Polarography, amperometric and bio-amperometric titrations.	**5**
5.	**Nuclear methods:** Fundamentals of radioactivity and decay, preparation of radioisotopes for tracers, applications with radiotracers, radiometric titration, radioactivity measurements by gas filled and scintillation detectors.	**6**
6.	**Solvent extraction**. Partition law and its limitations, distribution ratio, separation factor, factors influencing extraction, multiple extractions. Extraction of metal chelates.	**5**
7.	**Basic chromatography:** Introduction and classification, theory of column chromatography, retention time, retention volume, capacity factor, concept of plate and rate theory, resolution, column performance, normal and reverse phase chromatography, paper and thin layer chromatography, ion-exchangers.	**9**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/Books/ Publishers	Year of Publication/ Reprint
1.	Ewing, G.W., "Instrumental Methods of Chemical Analysis", 5th Ed. McGraw Hill.	**2004**

2.	Mendham, J., Denny, R.C., Barnes, J.D. and Thomas, M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed. Pearson Education.	**2004**
3.	Christian, G.D., "Analytical Chemistry" 6th Ed. Wiley	**2008**
4.	Sood, D.D., Reddy, A.V.R. and Ramamoorthy, N., "Fundamentals of Radiochemistry", IANCAS, BARC, Mumbai.	**2004**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-507** Course Title: **Structure and Reactivity of Organic Molecules**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs**)** **Theory: 3** **Practical: 0**

4. Relative weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PCC**

8. Pre-requisite: Nil

9. Objective of Course: To impart the knowledge of structure-reactivity and the reaction mechanism.

10. Details of Course

S. No.	Contents	Contact Hours
1.	**Conformational analysis of cyclic systems:** Cyclohexane and its derivatives (mono-, di- and tri-substituted), fused (decalins) and bridged bicyclic systems, dynamic stereochemistry, conformational rigidity and mobility, quantitative correlation between conformation and reactivity, effect of conformation on the reduction of cyclic ketones, nucleophilic addition to carbonyl group (Cram, Karabatsos, Felkin-Ahn models, Cieplak effect), nucleophilic substitution on cyclohexane substrates, cyclohexane epoxide formation and opening, elimination reactions of cyclohexyl halides, acetate esters and related compounds, deamination of 2-amino-cyclohexanols, elimination vs substitution competition and neighboring group participation reactions of acyclic and cyclic molecules.	**12**
2.	**Physical organic chemistry:** Basic concepts, thermodynamic and kinetic requirements, rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, reactivity *vs* selectivity principle, Curtin-Hammett principle, microscopic reversibility, kinetic *vs* thermodynamic control.	**8**
3.	**Methods for elucidating mechanism:** Kinetic analyses of simple and complex reactions, steady state and saturation kinetics, isotope effects – primary and secondary isotope effects, steric and equilibrium isotope effects, solvent isotope effects, heavy atom isotope effects, substituent effects – origin (inductive, field, resonance, steric, solvent and polarizability). Hammett linear free energy relationship, substituent parameter (sigma), reaction constant (rho), use of Hammett plot for mechanism determination, deviation from linearity, inductive *vs* resonance effects -Taft parameters, nucleophilicity and nucleofugality, factors affecting nucleophilicity (basicity/acidity, solvation, polarizability and shape), Swain-Scott parameters, Edwards and Ritchie correlations, solvent effects - bulk and specific solvent effects, Grunwald-Winstein plots, Bronsted relationships , experiments for identifying mechanism (example Cannizzaro reaction), product and intermediate identification, common intermediate detection (example Ritter reaction and Beckmann fragmentation), trapping and competition experiments, isotope labeling, crossover experiments.	**16**
4.	**Catalysis:** Binding in transition state *vs* ground state, electrophilic catalysis, acid and base catalysis, nucleophilic, covalent, Bronsted acid base catalysis (general and specific, Bronsted catalysis law, Leffler law), Libido rule.	**6**

	Total	**42**

11. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication / Reprint
1.	Anslyn, E. V. and Dougherty, D. A., "Modern Physical Organic Chemistry", University Science Books.	**2006**
2.	Clayden, J., Greeves, N. and Warren, S., "Organic Chemistry", Oxford University Press.	**2012**
3.	Carey, F. A. and Sundberg, R. J., "Advanced Organic Chemistry", Part A: Structure and Mechanisms, 5th Ed., Springer.	**2007**
4.	Nasipuri, D., "Stereochemistry of Organic Compounds: Principles and Applications", New Age International.	**2014**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-509** Course Title: **Coordination Chemistry**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**

4. Relative Weightage**: CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits**: 3** 6. Semester**: Autumn** 7.Subject Area**: PCC**

8. Pre-requisite**:** Nil

9. Objective: To impart basic and advanced concepts of coordination chemistry.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Structure, bonding and properties of transition metal complexes:** Different types of ligands and coordination geometry (symmetry considerations), coordination number, isomerism (recapitulation), HSAB concept, thermodynamic stability, successive and overall stability constants, determination of stoichiometry (Job's method) and stability constants by spectrophotometric, potentiometric and polarographic methods, Irving-William series, chelate and macrocyclic effect.	**6**
2.	**Stereochemical aspects of coordination complexes:** Stereoisomerism in inorganic complexes, isomerism arising out of ligand and ligand conformation, chirality and nomenclature of chiral complexes, optical rotatory dispersion (ORD) and circular dichroism (CD).	**5**
3.	**Metal-ligand bonding:** Overview of crystal field and ligand field theories of 4-, 5- and 6-coordinated complexes, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral, square pyramidal, trigonal-bipyramidal and cubic complexes, measurement of CFSE (d^1 to d^{10}) in weak and strong ligand fields, Jahn-Teller distortion, nephelauxetic series, variation of lattice energy, ionic radii and heat of hydration across 1^{st} row transition metal ions.	**6**
4.	**Molecular orbital theory (MOT) of coordination compounds:** Composition of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ and π bonding, angular overlap model.	**7**
5.	**Electronic spectra of coordination compounds:** Energy states from spectral terms of d^n configurations, selection rules for ligand-field and charge transfer transitions in metal complexes, band intensities, factors influencing band widths, splitting of various terms, Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral d^n complexes, calculation of ligand field parameters, luminescence, phosphorescent complexes.	**7**
6.	**Magnetic properties of coordination compounds:** Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects (L-S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over phenomenon, spin admixed states, metal-metal direct spin interaction and super exchange spin-spin interaction through bridging	**11**

	ligands, ferromagnetic, anti-ferromagnetic, ferrimagnetic behaviour of transition metal compounds, effect of temperature on their magnetic properties, single molecule magnets.	
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/Books/Publishers	Year of Publication/ Reprint
1.	Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons.	**1999**
2.	Douglas, B.E., McDaniel,D.H. and Alexander, J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons.	**2001**
3.	Figgis, B.N., and Hitchman, M.A "Ligand Field Theory and Its Applications", Wiley Eastern Ltd.	**1999**
4.	Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education, Inc.	**2003**
5.	Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., "Shriver and Atkins' Inorganic Chemistry", 4th Ed, Oxford university press.	**2009**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-511** Course Title: **Laboratory-I**

2. Contact Hours: **L: 0** **T: 0** **P: 12**

3. Examination Duration (Hrs): **Theory 0** **Practical 12**

4. Relative Weightage**: CWS: 0 PRS: 50 MTE: 0 ETE: 0 PRE: 50**

5. Credits: **6** 6. Semester**: Autumn** 7. Subject Area**: PCC**

8. Pre-requisite: Nil

9. Objective: To impart practical knowledge and skills in physical, inorganic and organic chemistry laboratories.

10. Details of Course:

Contents	Contact Hours
List of Inorganic Chemistry Experiments 1. Semi-micro qualitative analysis involving 6 radicals including interfering radicals. 2. Determination of metal ions by gravimetric-cum-volumetric analysis: Ag (I) gravimetrically and Cu(II) volumetrically. 3. Determination of Cu(II) gravimetrically and Zn(II) volumetrically. 4. Determination of Fe(III) gravimetrically and Ca(II) volumetrically. 5. Gravimetric analysis of a mixture of two metal ions such as Cu and Zn. 6. Synthesis of coordination compounds and metal content determination: (i) $[Cu(NH_3)_4.H_2O]SO_4$, (ii) $[Fe(acac)_3]$, (iii) $[Mn(acac)_3]$, (iv) $[Mn(C_2O_4)_3]$. • Some experiments require two-three turns.	**4 × 14**
List of Physical Chemistry Experiments 1. Determination of pK_1 and pK_2 of an acid using pH meter. 2. Determination of cell constant and verification of Kohlrausch's law. 3. Determination of specific rotation of lactic acid/sucrose by polarimeter. 4. Determination of molar refraction equivalent to $–CH_2$, C, H, and O. 5. Determination of composition of liquid mixture by refractive index measurements. 6. Determination of dimerization constant of benzoic acid. 7. Conductometric titration of different acids against bases. 8. Verification of Ostwald's dilution law by conductometric measurements of acetic acid. 9. Verification of Freundlich's adsorption isotherms and calculation of characteristic constants. 10. Verification of Langmuir adsorption isotherms and determination of surface area. 11. Determination of surface excess concentration and thickness of interfacial adsorbed layer by surface tension measurements of water-n-butanol mixture. 12. Determination of the Parachor of binary mixture of miscible solute by surface tension measurements. 13. Verification of Hardy-Schultze rule for positive/negatively charged colloids. 14. Determination of critical micelle concentration of sodium dodecylsulphate/cetyltri-	**4 × 14**

methylammonium bromide by surface tension method.	
List of Organic Chemistry Experiments 1. Separation of organic mixtures by TLC and PTLC. 2. Synthesis of derivatives for carbonyl, amino and active methylene compounds. 3. Diels-Alder reaction between anthracene and maleic anhydride. 4. Oxidation of hydroquinone to *p*-benzoquinone. 5. Oxidation of benzoin to benzil. 6. Conversion of benzil to quinoxaline. 7. Reduction of camphor. 8. Synthesis of 2-iodobenzoic acid by Sandmeyer reaction 9. Aldol condensation (benzaldehyde + acetone or cinnamaldehyde + acetone). 10. Synthesis of binaphthol by green reaction. 11. Knoevenagel condensation between aldehyde (4-diethylaminobenzaldehyde) and malonic acid, cyanoacetic acid or malononitrile. 12. Friedel-Crafts reaction: synthesis of 1,4-di-*tert*-butyl-2,5-dimethoxybenzene. 13. Preparation and purification of *cis*- and *trans*-stilbenes by Wittig reaction. 14. Bromination of acetanilide.	**4 × 14**
Total	**168**

11. Suggested Books:

S. No.	Authors/ Title/ Publisher	Year of Publication/Reprint
1	Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J., " Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., ELBS Longman Group UK Ltd.	**2004**
2	Srivastava T.N. and Kamboj P.C., "Analytical Chemistry", Vishal Publications.	**2000**
3	Furniss B.S., Handford A.J., Smith P.W.G. and Tatchell A.R., "Vogel's Text Book of Practical Organic Chemistry", 5th Ed., Longman.	**1996**
4	Leonard J., Lygo B. and Procter G., "Advanced Practical Organic Chemistry", Chapman & Hall.	**1995**
5	Levitt, B.P., "Findlay's Practical Physical Chemistry", 9th Ed., Longman	**1973**
6	Garland C.W., Nifler J.W. and Schoemaber D.P., "Experiments in Physical Chemistry", 7th Ed., McGraw-Hill International.	**2002**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-502** Course Title: **Organometallics, Inorganic Chains and Clusters**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**

4. Relative Weightage**: CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits**: 3** 6. Semester**: Spring** 7.Subject Area**: PCC**

8. Pre-requisite**:** Nil

9. Objective: To impart advanced concepts in organometallic chemistry and structural aspects of inorganic chains, rings, cages and clusters.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Structure and bonding in organometallics:** 18 electron rule and its application to π-acceptor ligands, limitations of 18 electron rule, description of bonding models for π-acceptor ligands including CO, alkenes (Dewar-Chatt-Duncanson model) and tertiary phosphines, physical evidences and consequences of bonding. Main group organometallics: Introduction, review of comparative aspects of synthetic methods, reactivity and bonding in ionic, covalent, electron deficient and electron rich organometallic compounds. Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands.	**9**
2.	**Organotransition metal chemistry:** σ-Bonded transition metal-alkyls, - aryls, -alkenyls(vinyls), -alkynyls(acetylides), reactions in σ–organyls: homolytic cleavage, reductive elimination, electrophilic cleavage, insertion, β-metal hydrogen elimination, α-abstraction or α-elimination and γ- and δ-remote C-H functionlization.	**5**
3.	**Organotransition compounds with multiple metal-carbon bonding:** Transition metal-carbenes/-carbynes, -bridging carbenes/carbynes, reactions of carbene/carbyne complexes such as ligand substitution, nucleophilic, electrophilic attack, dismutation, and ligand coupling reactions.	**4**
4.	**Organotransition compounds with multicenter bonds:** Concept of hapticity, transition metal complexes of alkenes, Ziese salt, alkynes, allyls, butadienes; π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cyclohepta-trienyls and cyclooctatetraenes, reactions and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxionalty, bimetallic and cluster complexes.	**6**
5.	**Inorganic chains, rings, cages and clusters:** Chains– catenation and hetero-catenation, structural aspects of silicate minerals and silicones, one-dimensional conductors: $(SN)_x$ chains, chalcogenide glasses, iso- and heteropolyanions. Rings–borazines, boron nitride, phosphazenes–structural models, phosphazene polymers, and other homocylic and heterocyclic inorganic ring systems. Cages– Boron cage compounds– structural aspects (boranes-styx number and Wade's rule) of higher boranes, carboranes, metallacarboranes, phosphorous cage compounds with P–P, P–O, P–S. Clusters– metal clusters, metal carbonyl clusters, di-, tri-, tetra- and	**14**

	hexanuclear clusters.	
6.	**Applications of organometallics and clusters in catalysis:** Alkene metathesis, Cativa and Monsanto processes for production of acetic acid, carbonylation and decarbonylation reactions, Wacker process, cyclooligomerisation of acetylene using Ni/Cr catalysts, Mobil and Fischer-Tropsch processes, polymer-bound catalysts, metal carbonyl clusters in catalysis.	**4**
	Total	**42**

11. Suggested Books:

S. No.	**Name of Authors/Books/Publishers**	**Year of Publication/ Reprint**
1.	Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education Inc.	**2003**
2.	Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons.	**1999**
3.	Hill, A.F., "Organotransition Chemistry", The Royal Society of Chemistry, Cambridge.	**2002**
4.	Bochmann, M. (Ed.), "Oxford Premier Series on Organometallics", Vol. 1 and 2, Oxford Press.	**2002**
5.	Gupta, B.D. and Elias A.J., "Basic Organometallic Chemistry", 2nd Ed., University Press (India) Pvt. Ltd.	**2013**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-504** Course Title: **Kinetics and Photochemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory: 3** **Practical: 0**
4. Relative weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PCC**
8. Pre-requisite: Nil
9. Objective of Course: To impart basic knowledge of the kinetics and photochemistry.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Theories:** Theoretical calculation of energy of activation using potential energy surface diagram, absolute reaction rate theory, comparison between gas phase and solution reactions.	**10**
2.	**Type of reactions:** Kinetics of chain reactions, detections of radical and kinetics of HBr, H_2O_2 reactions, explosion limits, elementary idea of unimolecular reactions, application of following to the reaction kinetics− solvent effect, kinetic isotope effect and salt effect, experimental technique for studying the fast reaction kinetics, kinetics of homogenous and heterogenous catalysis, kinetics of polymerization.	**14**
3.	**Electron transfer dynamics:** Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, experimental results, electron transfer in heterogeneous systems, electrode-solution interface, rate of charge transfer in electrode reactions, study of kinetics of electrode processes.	**8**
4.	**Photochemistry:** Quantum efficiencies of photochemical and photophysical processes, experimental techniques for continuous photolysis. Primary and secondary photochemical processes, Franck-Condon principle and its applications, rates of absorption and emission, lifetimes of electronically excited states and their fate, quenching of excited states species – dynamic and static quenching, radiationless transition and pre-dissociation, energy transfer processes, FRET analysis, mechanistic analysis and reaction dynamics. Radiation chemistry–Interaction with ionizing radiation with matter, dosimetry, generation of free radicals and intermediates, comparison between photo- and radiation chemistry.	**10**
	Total	**42**

11. Suggested books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/Reprint
1.	Laidler, K.J., "Reaction Kinetics", Anand Sons, New Delhi.	**2005**
2.	Amis, E.S.,"Solvent Effect of Reaction Rates and Mechanism", Academic Press.	**2005**
3.	Mukherjee, K.K., "Fundamentals of Photochemistry", New Age	**2004**

	International Pvt. Ltd., New Delhi.	
4	Lakowicz, J.R., "Principles of Fluorescence Spectroscopy", Plenum Press, New York.	**2003**
5.	Wishart, J.F. and Nocera, D.G., "Photochemistry and Radiation Chemistry", Oxford University Press, USA.	**1998**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-506** Course Title: **Organic Reaction Mechanisms**

2. Contact Hours: **L: 3 T: 0 P: 0**

3. Examination Duration (Hrs**): Theory: 3 Practical: 0**

4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PCC**

8. Pre-requisite: Nil

9. Objective of Course: To familiarize the students with different types of organic reactions.

10. Details of Course

S. No.	Contents	Contact Hours
1.	**Single bond [C-X (X = C, O, N)] formations:** Nucleophilic additions to carbonyls and stereochemical aspects through various models (Cram, Cram chelation and Felkin-Anh models), chemistry of enolates (kinetic and themodynamic) and enamines, enolates, lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates, mechanism of aldol (Mukiyamaaldol), Knoevenagel, Claisen, Dieckmann, Perkin, Stobbe, Darzen, Acyloin condensations, organolithium, organomagnesium (Grignard), organozinc, organocopper (Gilman &Normant) reagents in synthesis, epoxidations (Prilezhaev, Sharpless, Jacobsen and Shi), Metal catalyzed C-C bond formations (Ullmann, Buchwald-Hartwig, Sonogashira, Heck, Suzuki, Stille, Nozaki-Hiyama and Kumada reactions).	**14**
2.	**Multiple bond [C-X (X = C, N)] formations:** Phospohorus, nitrogen and sulfur ylids, Wittig reaction, Wittig-Horner reaction, Tebbe olefination, Julia olefination, Robinson annulation, Mannich reaction, Peterson olefination, Ramberg-Backlund rearrangement, McMurry reaction, Shapiro reaction, β-eliminations (Hoffman & ester pyrolysis), Cope elimination, selenoxide elimination, dehydration of alcohols, Corey-Winter reaction, olefins from epoxides, reduction of acetylenes, olefin metathesis (Schrock's catalyst, Grubbs' catalyst), ring closing metathesis, enyne metathesis, Thorpe reaction, Corey-Fuchs reaction, Seyferth-Gilbert homologation, Ohira-Bestmann modification.	**14**
3.	**Pericyclic reactions:** Classification, electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, conservation of orbital symmetry, state correlation diagrams, frontier molecular orbital (FMO) theory, aromatic transition state (ATS) theory, generalized orbital symmetry (GOS) rule, photochemical cycloaddition reactions, Diels-Alder reaction, Dipolar cycloadditions, retrocycloadditions, electrocyclic reactions, conrotation and disrotation, orbital correlation diagrams for four-, six- and eight-electron cases, torquoselectivity, sigmatropic rearrangements, [1,3], [1,5] and [3,3] shifts, Curtius and Schmidt rearrangements, Cope and Claisen rearrangements, di-π-methane rearrangement, ene reaction, cheletropic reactions, Norrish I and II reactions.	**14**
	Total	**42**

11. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication / Reprint
1.	Carey, F. A. and Sundberg, R. J., "Advanced Organic Chemistry, Part B: Reactions and Synthesis", 5th Ed., Springer.	**2007**
2.	Anslyn, E. V. and Dougherty, D. A., "Modern Physical Organic Chemistry", University Science Books.	**2006**
3.	Clayden, J., Greeves, N. and Warren, S., "Organic Chemistry", Oxford University Press.	**2012**
4.	Smith, M.B., "Organic Synthesis", 3rd Ed., Academic Press.	**2010**
5.	Bruckner, R., "Organic Mechanisms: Reactions, Stereochemistry and Synthesis", Springer.	**2010**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-508** Course Title: **Molecular Spectroscopy**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**
4. Relative Weightage**: CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**
5. Credits**: 3** 6. Semester**: Spring** 7. Subject Area**: PCC**
8. Pre-requisite**:** CYN-501; Elementary knowledge of symmetry and group theory.
9. Objective: To provide advance knowledge of spectroscopic techniques for identification and elucidation of structures of molecules.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Overview of molecular spectroscopy:** Different aspects of molecular spectroscopy, the Born-oppenheimer approximation, transition probability, oscillator strength, the integrated absorption coefficient. **Microwave spectroscopy:** Classification of the rotors, intensity of the rotational lines, population of energy levels, non-rigid rotation, anharmonicity and centrifugal distortion, effect of isotopic substitution. Rotation spectra of the linear, spherical top and asymmetric top polyatomic molecules, microwave technique.	**6**
2.	**Infrared and Raman spectroscopy:** Types of vibration bands- overtones, combination bands, Fermi resonance phenomenon, the finger print region, FTIR spectroscopy and application. Rayleigh and Raman scattering, polarizabilities, rotational and vibrational Raman spectra, selection rules, polarization of the light and Raman effect, resonance Raman and coherent anti-Raman spectroscopy.	**6**
3.	**UV-visible spectroscopy:** Electronic spectra, Frank-Condon Principle, predissociation spectra, Fortrat diagram, conjugated polyene and enone systems, different types of charge transfer transitions and their basis. Charge transfer spectra in organic and inorganic systems.	**5**
4.	**Photoelectron spectroscopy:** The photoionization processes, Auger and autoionization processes, deexcitaion by fluorescence, outlines of UPS, XPS and Auger techniques and their applications in interpretation of valence and core shell spectra of atoms and molecules.	**4**
5.	**Magnetic resonance spectroscopy:** Nuclear moments, nuclear spin states in a magnetic field and the resonance phenomenon, relaxation processes and their importance. Bloch equation, Larmor frequency, shielding constant and chemical shifts. Spin-spin coupling and quantum chemical description of spin systems-- spectra of two (AX cases) and three (AMX) spin systems. Dynamic NMR and line shapes. General introduction to double resonance experiments and nuclear overhauser effect, chemical shift reagents, multinuclear NMR. **ESR Spectroscopy:** Principle of ESR and interpretation of its applications for ESR spectra of -CH_3 and –CH_2 radicals.	**14**
6.	**Mössbauer spectroscopy:** The Mössbauer effect and chemical isomer shift. Magnetic and quadrupolar effects in the Mössbauer spectra of complexes of ^{57}Fe and other nuclei.	**6**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/Reprint
1.	Banwell, C.N. and McCash, E.L.M.,"Fundamentals of Molecular Spectroscopy", 4th Ed. McGraw-Hill N. Y.	**1999**
2.	Slichter, C.P., " Principles of Magnetic Resonance", Springer Verlag.	**1981**
3.	Graybeal, J.D., "Molecular Spectroscopy", McGraw-Hill.	**1988**
4.	Atkins, P. and Paula, J.de, "Physical Chemistry", 7th Ed., Oxford Univ. Press.	**2003**
5.	Drago, R.S., "Physical Methods in Inorganic Chemistry", Reinhold Publishing Corp., East West Press Ltd.	**1986**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-510** Course Title: **Laboratory-II**

2. Contact Hours: **L: 0** **T: 0** **P: 12**

3. Examination Duration (Hrs): **Theory 0** **Practical: 12**

4. Relative Weightage**: CWS: 0 PRS: 50 MTE: 0 ETE: 0 PRE: 50**

5. Credits: **6** 6. Semester**: Spring** 7. Subject Area**: PCC**

8. Pre-requisite: CYN-511

9. Objective: To impart practical knowledge and skills in physical, inorganic and organic chemistry laboratories.

10. Details of Course:

Contents	Contact Hours
List of Inorganic Chemistry Experiments 1. Comparison of the electronic spectra of $[Ni(H_2O)_6]^{2+}$, $[Ni(NH_3)_6)^{2+}$ and $[Ni(en)_3]^{2+}$ and qualitative verification of the spectrochemical series, and quantitative estimation of nickel by spectrophotometry. 2. Synthesis and spectrophotometric study of copper complexes: (i) synthesis of bis(salicylaldimine)copper(II) and cis-bis(glycinato)copper(II), (ii) record the spectra of bis(salicylaldimine)copper(II) and cis-bis(glycinato copper(II), and (iii) record spectra of Cu^{2+} in water, NH_3, ethylene diamine and glycine, and arrange the ligands in order of increasing field strength and (iv) quantitative estimation of copper by spectrophotometry. 3. (i) Study of the complex formation between Fe(III) and thiocyanate/salicylic acid/sulphosalicylic acid or between Ni(II) and *o*-phenanthroline, and (ii) spectrophotometric determination of formation constant of the complex (Job's method and molar ratio method). 4. Preparation of (i) $[Ni(NH_3)_6]Cl_2/SO_4$, (ii) $[Ni(en)_3]Cl_2/SO_4$, (iii) bis(salicylaldimine)nickel(II), and analysis by different methods, viz. IR, UV-visible and ^1H NMR spectroscopy. 5. Synthesis of potassium tris(oxalato)aluminate, potassium tris(oxalato)chromate and potassium tris(oxalato)ferrate, and their characterization by metal determination, various spectroscopic (I.R. and U.V.-Vis) methods, magnetic moment determination, and photochemical behavior of iron complex. 6. Synthesis and characterization of $[Co(en)_3]Cl_3$. Separation of its optical isomers and determination of their optical rotation by using polarimeter. • Some experiments require two-three turns.	**4 × 14**
List of Physical Chemistry Experiments 1. To study the kinetics of H^+ catalyzed hydrolysis of an ester. 2. To study the kinetics of saponification of an ester. 3. To study the kinetics of Fe^{3+} catalyzed decomposition of hydrogen peroxide. 4. To study the kinetics of inversion of sucrose using polarimeter. 5. Determination of equilibrium constant of KI_3 complex by distribution method. 6. Determination of compound formation between liquids by viscosity variation with composition of mixtures of liquids using Ostwald viscometer.	**4 × 14**

7. Determine the composition of KCl-KBr mixtures by potentiometric titration against silver nitrate solution. 8. Verification of Beer-Lambert's law using potassium permanganate solution. 9. To study the quenching of fluorescence of organic dye(s). 10. To study the variation in miscibility of phenol in water with temperature and to find out the critical solution temperature (CST) and also to investigate the effect of impurity on CST. 11. To determine the molecular weight of a volatile substance using Victor Meyer method. 12. To determine the cell potentials for different electrochemical cells and also to measure different thermodynamic parameters. • Some experiments require two turns.	
List of Organic Chemistry Experiments 1. Preparation of *p*-nitroaniline from acetanilide. 2. Preparation of pyridinium dichromate and its use in oxidation of benzyl alcohol. 3. Cannizzaro reaction of an aromatic aldehyde (*p*-nitrobenzaldehyde). 4. Synthesis of ω-nitrostyrene from an aromatic aldehyde and nitromethane. 5. Synthesis of chalcone from an aromatic aldehyde and acetophenone. 6. Extraction of oils from ground nuts using soxhlet apparatus. 7. Synthesis of α-bromo cinnamic acid or phenyl acetylene from benzaldehyde, (formation of cinnamic acid, bromination and elimination reactions). 8. Preparation of *meso*-stilbene dibromide and its conversion to diphenylacetylene. 9. Fisher indole synthesis. • Some experiments require two-three turns.	**4 × 14**
Total	**168**

11. Suggested Books:

S. No.	Authors/ Title/ Publisher	Year of Publication/Reprint
1	Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J., " Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., ELBS Longman Group UK Ltd.	**2004**
2	Srivastava T.N. and Kamboj P.C., "Analytical Chemistry", Vishal Publications.	**2000**
3	Furniss B.S., Handford A.J., Smith P.W.G. and Tatchell A.R., "Vogel's Text Book of Practical Organic Chemistry", 5th Ed., Longman.	**1996**
4	Leonard J., Lygo B. and Procter G., "Advanced Practical Organic Chemistry", Chapman & Hall.	**1995**
5	Levitt, B.P., "Findlay's Practical Physical Chemistry", 9th Ed., Longman	**1973**
6	Garland C.W., Nifler J.W. and Schoemaber D.P., "Experiments in Physical Chemistry", 7th Ed., McGraw-Hill International.	**2002**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject code: **CYN-5 12** Course Title: **Nuclear and Radiochemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**
4. Relative Weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PEC**
8. Pre-requisite: Fundamental knowledge in physical chemistry.
9. Objective: To impart basic knowledge in nuclear chemistry and apply its concepts for characterization of materials and analysis.
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Properties of nucleons and nuclei:** Nuclear stability and natural radioactivity, size and shape of a nucleus, nuclear spin, magnetic properties of a nucleus, nuclear magnetic resonance, nuclear resonance or recoil-less absorption, electric quadrupole moment, nuclear parity and nuclear statistics.	**6**
2.	**Nuclear models:** Shell model, liquid drop model, Fermi gas model, collective model and optical model.	**4**
3.	**Radioactivity**: Radioactive decay, decay kinetics, parent daughter decay growth relationship, concepts of transient and secular equilibrium, alpha, beta and gamma decay, artificial radioactivity.	**6**
4.	**Nuclear reaction:** Bethe's notation, types of nuclear reaction, reaction cross section, Q- value and threshold, compound nucleus theory, transuraniens, photo and thermonuclear reaction, fusion reactor, nuclear fission, fission fragments and mass distribution, fission energy, theory of nuclear fission, introduction to nuclear reactor and importance of four factor formula, reprocessing of spent fuels, nuclear waste management.	**8**
5.	**Interaction of radiation with matter:** Stopping power and range for charged particles, interaction with X-rays and gamma rays – photoelectric effect, Compton scattering, pair production, nuclear detectors using semiconductors, effect of radiation on polymers and inorganic compounds, concepts of positron and its use in materials science.	**10**
6.	**Ion beam techniques:** Activation analysis with case studies, radioisotopes for nuclear medicine, elemental mapping of trace and major elements, depth wise analysis by RBS, elastic recoil deflection analysis for hydrogen measurement, ion implantation, ion beam mixing.	**8**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/Books/ Publishers	Year of Publication/ Reprint
1.	Loveland, W., Morrissey and D., Seaborg, G.T., "Modern Nuclear Chemistry", John Wiley and Sons, New Jersey.	**2006**
2.	Arnikar, H.J.,"Essentials of Nuclear Chemistry", New Age International (P) Ltd., New Delhi.	**2003**
3.	Friedlander, G., Kennedy J.W., Miller, E.S. and Macais, J.M., " Nuclear and Radiochemistry", John Wiley and Sons, Inc. New York.	**1981**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-514** Course Title: **Heterocyclic Chemistry**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs) **Theory: 3** **Practical: 0**

4. Relative weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PEC**

8. Pre-requisite: Basic organic chemistry and synthetic methods.

9. Objective of Course: To impart a broad understanding of the major classes of 5- and 6-membered ring heterocyclic compounds.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Heterocycles:** Systematic nomenclature of heterocyclic compounds (Hantzsch-Widman, replacement and fusion methods), biological importance of heterocyclic compounds.	**2**
2	**Five-membered heterocycles with one heteroatom:** Chemical structures of furan, pyrrole and thiophene, and degree of aromaticity. General syntheses methods for 5-member rings. Paal-Knorr, Feist-Benary, Hantzsch and Knorr syntheses. Electrophilic substitution, reactants employed and orientation of the substituent on the ring.	**10**
3	**Benzo derivatives of five-membered heterocycles with one heteroatom:** Preparation of indole and carbazole derivatives. Fisher, Bischler, Madelung and Reissert syntheses. Preparation and reactivity of benzofurans (coumarins), benzothiophenes, dibenzofurans and dibenzothiophenes.	**8**
4.	**Pyridines, quinolines and isoquinoles:** Influence of the imine group on the reactivity of the pyridine ring. Nucleophilic and electrophilic substitutions on pyridine, quinolines and isoquinolines. Comparison of reactivity with benzene and naphthalene. Preparation of pyridine salts and pyridine *N*-oxides and synthetic applications. Skraup, Friedlander, Pfintzinger Bischler-Napieralski and Pictet syntheses.	**10**
5.	**Heterocycles with 5 or 6 members and two or three heteroatoms:** Syntheses and reactivity of **o**xazoles, thiazoles, oxadiazoles, thiadiazoles, benzothiazoles, benzothiadiazoles, triazole, benzotriazole, pyrimidines, pyrazines, quinoxalines and triazines	**6**
6.	**New materials derived from heterocycles:** Syntheses of indigo, mauveine, cyanines, tetrathiafulvalenes and related dyes, organic sensitizers for DSSC, electron donors and acceptors for organic solar cells, optical chemosensors and organic semiconductors for thin-film transistors.	**6**
	Total	**42**

11. Suggested Books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Gilchrist, T. L.,"Heterocyclic Chemistry", 3rd Ed., Pearson Education, India. (ISBN: 978-0582278431).	**2007**
2.	Sainsbury, M., "Heterocyclic Chemistry", Wiley. (ISBN: 978-0-471-28164-1)	**2002**
3.	Katritzky ,A. R., Ramsden, C. A., Joule, J. A. and Zhdankin, V. V., "Handbook of Heterocyclic Chemistry", 3rd Ed., Elsevier. (ISBN: 978-0-08-095843-9)	**2010**
4.	Gupta, R. R., Kumar, M. and Gupta, V., "Heterocyclic Chemistry, Vol. I: Principles, Three- and Four-Membered Heterocycles", Springer. (ISBN: 978-3-642-72278-3)	**1998**
5.	Gupta, R. R., Kumar, M. and Gupta, V., "Heterocyclic chemistry, Vol. II: Five-Membered Heterocycles", Springer. (ISBN: 978-3-642-08460-7)	**1998**
6.	Joule, J. A. and Mills, K., "Heterocyclic Chemistry", Wiley-Blackwell. (ISBN: 978-1-4051-3300-5)	**2010**

It has been passed by Senate and there is no change in the contents of the course except the course no. has been changed.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-516** Course Title: **Chemistry of Main Group and Transition Elements**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**

4. Relative Weightage**: CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits**: 3** 6. Semester**: Spring** 7.Subject Area**: PEC**

8. Pre-requisite**:** Basic knowledge of inorganic chemistry.

9. Objective: To impart advance concepts in chemistry of main group and transition elements.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Chemistry of main group elements:** (i) Chemistry of Gr. 1 and 2 metals– solutions of alkali metals in liquid ammonia (reactions, electrical and magnetic properties), metal anions, complexation of Gr. I/II metals with crown ethers, cryptands and calixarenes, anomalous behavior of Li and Be. (ii) Chemistry of *p*-block elements– borides, borates and boran halides, allotropes of carbon (diamond, graphite, fullerene, carbon nanotubes), carbides, chlorofluorocarbons, silicon halides, silanes, silanols. Hydrides, oxides and oxoacids of pnictogens (N, P), chalcogens (S, Se and Te) and halogens. Pseudohalogens, inter-halogens, polyhalide anions, synthesis, structures and reactivity of compounds of xenon, bonding in xenon fluorides. Overall structural and bonding aspects (VBT) of B, Al, Si, N, P and Cl compounds.	**14**
2.	**Types of non-covalent interactions:** Inter- and intramolecular hydrogen bonding interactions and their effects, electrostatic interactions (ion-ion, ion-dipole, dipole-dipole, dipole-induced dipole) and other weak intermolecular forces. Principle of self-assembly, host-guest chemistry and molecular receptors, examples of supramolecular inorganic architectures, and supramolecular photochemistry. Metallic Bonding– band model, soft X-ray spectra and N(E) curves, binding energy in metals, conductors, semiconductors and insulators, effect of temperature and impurity on conductivity.	**7**
3.	**Concept of acid and bases**: Bronsted and Lewis acids and bases, pH, pKa, acid - base concept in non-aqueous media, buffer solution, protonic acids, proton affinities, differentiation and leveling solvents, Hammet Ho scale, acidic behavior of the binary hydrides, cosolvating agents, oxyacids. aquoacids, amphoteric oxides, nonprotonic concepts of Acid - Base reactions, Lux concept, solvent ion theory of acids and bases, non-aqueous solvents– liquid ammonia, acetic acid, BF_3. Hard and soft acids and bases, symbiosis, theoretical and electronegativity concepts of hardness and softness.	**7**
4.	**Lanthanides and actinides:** Separation and isolation of lanthanides, separation of Np, Pu and Am from U, electronic spectra and magnetic properties of lanthanides and actinides, general comparison of lanthanides and actinides and their applications in technology, lanthanide shift reagents.	**6**
5.	**Introductory bioinorganic chemistry:** Inorganic composition of cells, compartmentalization, classification of biomolecules, biological metal-coordination	**8**

	sites including special ligands like porphyrins and pterin. Role of metallobiomolecules in transport, transfer and transcription (preliminary ideas), selective transport and storage of iron. Chemistry of elements in medicine–chelation therapy, cancer treatment, imaging agents, anti-arthritis agents, radioisotopes and contribution of individual elements. Electron transfer proteins - active site structure and functions of ferredoxin, rubridoxin and cytochromes, and their comparisons. Mechanism of nitrogen fixation.	
	Total	**42**

11. Suggested Books:

S. No.	**Name of Authors/Books/Publishers**	**Year of Publication/ Reprint**
1.	Huheey, J. E., Keiter, E. A. and Keiter, R. L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education, Inc.	**2003**
2.	Douglas, B.E., McDaniel, D.H. and Alexander, J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons.	**2001**
3.	Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons.	**1999**
4.	Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F. "Shriver and Atkins' Inorganic Chemistry", 4th Ed, Oxford University Press.	**2009**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-518** Course Title: **Structure, Bonding and Properties of Solids**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs): **Theory 3** **Practical 0**

4. Relative Weightage**: CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester**: Spring** 7. Subject Area**: PEC**

8. Pre-requisite: Nil

9. Objective: To impart fundamental understanding of crystal structure, bonding and physical properties of solids.

10. Details of Course:

Sl. No.	Contents	Contact Hours
1.	**Symmetry in the crystalline state:** Crystal symmetry, elements of translation-screw axis and glide planes, symmetry in a cube, crystal classes, stereographic projection of crystal systems, space symmetry and space groups, Hermann-Mauguin and Schoenflies notations, Wyckoff positions, representation of monoclinic and orthorhombic space groups.	**8**
2.	**X-Ray diffraction:** Crystal planes and directions, Bragg's law in reciprocal space and Ewald sphere, structure factor, integrated intensity and systematic absences/presences, indexing and simulation of powder X-ray diffraction patterns for simple systems.	**8**
3.	**Crystal chemistry**: Hard sphere model, structures derived from HCP and CCP packing, crystal structures of various compositions, derived structures and polytypes, non-stoichiometry in solids, atomic order/disorder in solids, single crystals, polycrystals, quasicrystals, amorphous / glassy solids.	**8**
4.	**Bonding in solids:** Bonding in molecular solids – polymorphism, bonding in extended solids - ionic, covalent and metallic. Band theory of solids - classification of semiconductors, metals and insulators, free electron theory, Bloch's theorem, concept of density of state and elementary band theory, band structures of one-, two- and three- dimensional solids, selected metals and insulators.	**8**
5.	**Properties of solids:** Thermal, electrical, magnetic and dielectric properties of solids.	**10**
	Total	**42**

11. Suggested Books:

Sl. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	West, A. R., "Solid State Chemistry and its Applications", Reprint, Wiley India.	**2013**
2.	Rao, C.N.R. and Gopalakrishnan, J., "New Directions in Solid State Chemistry", 2nd Ed., Cambridge University Press.	**1997**
3.	Stout, G.H. and Jensen, L.H., "X-Ray Structure Determination: A Practical Guide", 2nd Ed., Wiley-Interscience.	**1989**
4.	Giacovazzo, C., Artioli, G. and Monaco, H. L., "Fundamentals of Crystallography", Oxford University Press.	**2006**
5.	S. Nicola, "Magnetic Materials: Fundamentals and Device Applications", Cambridge University Press.	**2003**
6.	Cox, P. A., "The Electronic Structure and Chemistry of Solids", Oxford University Press.	**1987**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-601** Course Title: **Laboratory-III**

2. Contact Hours: **L: 0** **T: 0** **P: 8**

3. Examination Duration (Hrs): **Theory 0** **Practical 8**

4. Relative Weightage**: CWS: 0 PRS: 50 MTE: 0 ETE: 0 PRE: 50**

5. Credits: **4** 6. Semester**: Autumn** 7. Subject Area**: PCC**

8. Pre-requisite: CYN-511 and CYN-510

9. Objective: To impart practical knowledge and skills in handling instruments in physical, inorganic and organic chemistry laboratories.

10. Details of Course:

Contents	Contact Hours
1. Separation of binary mixture of organic compounds using column chromatography. 2. Simultaneous spectrophotometric determination of concentration of $KMnO_4$ and $K_2Cr_2O_7$ in a given mixture. 3. Determination of Na, K in a soil sample by flame photometry. 4. Determination of metal in alloy samples by AAS. 5. Radiation measurement by GM counter. 6. Determination of metal ions by polarography and voltammetry methods. 7. Extraction of Fe^{3+} using 8-hydroxyquinoline. 8. Catalytic oxidation of organic substrates and analysis by GC. 9. Structure elucidation of organic molecules using ^{1}H and ^{13}C NMR spectra. 10. Synthesis, characterization and applications of ZnO or CdS or CdSe nanoparticles 11. Luminol synthesis from 3-nitrophthalic acid and chemiluminescence demonstration. 12. Preparation of anthracene from phthalic anhydride. 13. Esterification and nitration of *p*-hydroxybenzoic acid. 14. Synthesis of 4-cyano-2-aminophenol from 4-hydroxybenzaldehyde.	**8 × 14**
Total	**112**

11. Suggested Books:

S. No.	Authors/ Title/ Publisher	Year of Publication/Reprint
1	Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J., " Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., ELBS Longman Group UK Ltd.	**2004**
2	Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill.	**2004**
3	Furniss B.S., Handford A.J., Smith P.W.G. and Tatchell A.R., "Vogel's	**1996**

	Text Book of Practical Organic Chemistry", 5th Ed., Longman.	
4	Garland C.W., Nifler J.W. and Schoemaber D.P., "Experiments in Physical Chemistry", 7th Ed., McGraw-Hill International.	**2002**
5	Levitt, B.P., "Findlay's Practical Physical Chemistry", 9th Ed., Longman	**1973**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject code: **CYN-603** Course Title: **Advanced Analytical Techniques**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**
4. Relative Weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Nil
9. Objective: To impart knowledge of specialized topics in analytical chemistry.
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Electroanalytical methods:** Instrumentation, theory and applications of polarography−normal DC, pulse and differential pulse polarography, AC polarography. Linear and cyclic voltammetry, square wave voltammetry, coulometry at controlled potential, chronopotentiometry, anodic stripping voltammetry. Sensors−different types of solid and liquid sensors, nano material and chemically modified sensors, applications in environmental and biological sample analysis.	**14**
2.	**Nuclear and X-ray methods:** Radiotracers– choice and synthesis of radiotracers, isotope dilution methods, neutron activation analysis. Material science studies using positron emitters and Mössbauer source. Principles of X-ray spectra, X-ray absorption, emission fluorescence and diffraction methods and applications. Ion beam analysis, proton induced X-ray emission, Rutherford backscattering spectrometry, elastic recoil detection analysis for hydrogen measurement, nuclear microprobe.	**14**
3.	**Mass spectrometry**. Different types of ion sources, mass analyzers and detectors, resolution and resolving power, interpretation of mass spectra, hyphenated systems like LC-MS, GC-MS, MS-MS.	**8**
4.	**Atomic spectroscopy and hyphenation** Atomic absorption spectroscopy with electro thermal atomizers, cold vapor technique, inductively coupled plasma atomic emission methods − principle and instrumentation, hyphenation with mass spectrometry (ICP-MS), laser ablation and HPLC.	**6**
	Total	**42**

1. Suggested Books:

S. No.	Name of Authors/Books/ Publishers	Year of Publication/ Reprint

1.	Meites, L., "Polarographic Techniques", 3rd Ed., Interscience publishers, N.Y..	**1990**
2.	Sane, R.T. and Joshi, A.P., "Electroanalytical Chemistry: Theory and Applications", Quest Publications.	**1999**
3.	Loveland, W., Morrissey, D. and Seaborg, G.T., "Modern Nuclear Chemistry", John Wiley and Sons, New Jersey.	**2006**
4.	Sood, D.D., Reddy, A.V.R. and Ramamoorthy N., "Fundamentals of Radiochemistry", IANCAS, BARC, India.	**2004**
5.	Skoog, D.A., Holler, F.J. and Crouch, S.R., "Principles of Instrumental Analysis", Thomson Brooks/Cole, Canada.	**2007**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject code: **CYN-605** Course Title: **Separation Techniques and Microanalysis**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**
4. Relative Weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Nil
9. Objective: To impart knowledge of specialized topics in analytical chemistry.
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Chromatographic techniques:** Processes leading to non-ideal chromatography, extended form of Van Deemter equation, gas chromatography− instrumentation, types of column, stationary and mobile phases, detectors, Kovat's index, high pressure liquid chromatography− instrumentation, stationary and bonded-stationary phases, detectors, ion chromatography, size exclusion chromatography, supercritical fluid chromatography, affinity chromatography, electrophoresis.	**12**
2.	**Liquid – liquid extraction:** Principle, significance of various terms, batch and counter current extraction, classification of extraction systems, extraction equilibria of metal chelates, ion association extraction systems, extraction with high molecular weight amines, synergism, stripping, backwashing, salting out agents, masking agents, emulsion formation, identification of extracting species, analysis of organic phase, analysis of raffinate, environmental considerations, solid phase extraction.	**12**
3.	**Membrane and allied methods of separation:** Fundamentals and various terms, Liquid membranes, Cloud point extraction, Micellar enhanced separation processes, external field induced membrane separation processes.	**4**
4.	**Sample preparation techniques for analysis:** Extraction of semi-volatile organics from liquid, solid matrices, sample preparation for metal analysis, isoloation of nucleic acid for analysis, methods for preparing thin films for spectroscopic studies	**6**
5.	**Microfabrication, microanalysis and automation:** Photolithography, electron and ion beam lithography, microfluidics for analytical techniques used in micro-total analytical System (μTAS), automation in analytical methods,instrumental parameters for automated devices, principles and techniques of automation for microanalysis with emphasis on sequences of operational modes in segmented and continuous flow, non destructive autoanalysers, applications in environmental and clinical cases.	**8**

	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/Books/ Publishers	Year of Publication/ Reprint
1.	Rousseau, R.W.,"Handbook of Separation Process Technology", John Wiley & Sons.	**1989**
2.	Fifield, F.W. and Kealey, D., "Principles and Practice of Analytical Chemistry", 5th Ed., Blackwell Science.	**2000**
3.	Li, N.N., Fane, A.G., Winston, W.S. and Matsuura, H. T., (Eds.), "Advanced Membrane Technology and Applications", Wiley.	**2008**
4.	Mitra, S. (Ed.), "Sample preparation techniques in Analytical Chemistry", John Wiley and Sons, New Jersey.	**2003**
5.	Madou, M.J.," Fundamentals of Microfabrications and Nanotechnology", 3rd Ed., CRC Press.	**2011**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-607** Course Title: **Electroanalytical Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory: 3** **Practical: 0**
4. Relative weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Nil
9. Objective of Course: To introduce theoretical and practical knowledge of various electroanalytical systems.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Polarographic techniques:** Operational amplifiers concept and design of polarographic circuit using op-amps. Ilkovic equation, theory of diffusion, kinetic, adsorption and catalytic currents. Controlled potential electrolysis and coulometry. 2 and 3 electrodes systems. Polarography versus voltammetry, determination of number of electrons. Theory of reversible, quasi-reversible and irreversible electrode processes. Pulse and differential pulse polarography and their superiority over DC polarography. A.C. polarography.	**14**
2.	**Voltammetric techniques:** Linear and cyclic sweep voltammetry, Randles Sevcik equation, effect of sweep rate and evaluation of adsorption characteristics of reactant or product using CV. Coupled chemical reactions and their characterization. Characteristics of commonly used working electrodes such as glassy carbon, platinum, pyrolytic graphite and reference electrodes SCE and Ag/AgCl. Enzyme catalysed oxidations of biomoleules viz., uric acid, guanine, adenine and their comparison with electrochemical reactions. Anodic and cathodic stripping and determination of metal ions, pollutants and biomolecules using stripping voltammetry.	**14**
3.	**Sensors:** Amperometric and voltammetric sensors. Modified electrodes and their advantages over conventional electrodes in sensing variety of metals and biomolecules. Nanomaterials in electrode modification–C_{60}, single wall and multi wall carbon nanotubes. Preparation and characterization of modified surfaces. Applications of sensors in determining cases of doping.	**7**
4.	**Polarographic and cyclic voltametric studies of coordination compounds:** Compounds containing one or more redox centers, coupled chemical reactions — EE and EEE mechanisms, stability constant of complexes.	**7**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint

1.	Meites, L., "Polarographic Techniques", 3rd Ed., Interscience publishers, N.Y.	**1990**
2.	Lund and Baizer, "Organic Electrochemistry", Marcel Dekker, New York.	**2000**
3.	Bard, A.J. and Faulkner, L.R., "Electrochemical Methods-Fundamentals and Applications", John Wiley.	**2000**
4.	Sane, R.T. and Joshi, A.P., "Electroanalytical Chemistry: Theory and Applications", Quest Publications.	**1999**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-609** Course Title: **Inorganic Biochemistry and Reaction Mechanism**

2. Contact Hours: **L: 3 T: 0 P: 0**

3. Examination Duration (Hrs): **Theory: 3 Practical: 0**

4. Relative weightage**: CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: P**EC**

8. Pre-requisite: Knowledge of coordination chemistry.

9. Objective of Course: To familiarize the students with mechanisms of inorganic reactions and inorganic biochemistry.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Inorganic reaction mechanism:** Substitution reactions in octahedral complexes– exchange reactions, acid- and base-hydrolysis, annation reaction, solvolytic and catalysed reactions. Substitution reactions in square-planar complexes–effect of non-participation of ligands on reactivity, *cis* and *trans* effects.	**6**
2.	**Electron transfer reactions:** Outer- and inner-sphere mechanisms, factors affecting electron transfer reaction rates, theories of electron transfer reactions, solvated electron.	**5**
3.	**Photochemistry of metal complexes:** Introduction to inorganic photochemistry, photochemically excited states and excited state processes for transition metal complexes, photochemical reactions of coordination compounds (Cr and Ru complexes), types of photochemical reactions in transition metal complexes– substitution, decomposition, fragmentation, rearrangement and redox reactions. Mechanism of charge transfer (CT) to mass (CTTM) photoreduction. Applications of photochemical inorganic reactions in synthesis, catalysis, biological processes and in lasers.	**6**
4.	**Inorganic biochemistry:** Metalloproteins and enzymes– Role of metal ions in the active sites, structure and functions of metalloproteins and enzymes containing Mg, Ca, V, Mn, Fe, Co, Ni, Cu and Zn ions. Detailed structure and mechanistic studies of the following–Mn-photosystem-II, catalase, pseudocatalase, oxygen carriers, haemoglobin, myoglobin, non-porphyrin oxygen carriers, hemerythrin, hemocyanin, Fe-ribonucleotide reductase, cytochrome c oxidases, cytochrome P-450s, Ni-urease, hydrogenase, nitrogen fixation, Cu-blue copper protein, tyrosinase, galactose oxidase, superoxide dismutases, Zn-carbonicanhydrase, carboxypeptidase, alcohol dehydrogenase. Biological importance of Vitamin B_{12} and coenzymes, and their biomimetic studies.	**17**
5.	**Chemical toxicity and metallotherapy:** Toxic chemicals in the environment, toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens, metal containing drugs in therapy, interaction of heavy metal ions with DNA, DNA cleavage, structure-activity relationship and mode of action. Organometallic compounds as therapeutic drugs and enzyme inhibitors.	**8**
	Total	**42**

11. Suggested books:

S.No.	Name of Authors/Books/ Publishers	Year of Publication/ Reprint
1.	Huheey, J.E., Keiter, E. and Keiter, R., "Inorganic Chemistry: Principles of Structure and Reactivity", 4th Ed., Pearson Education Asia, 3rd Indian reprint.	**2001**
2.	Wilkins, R.G., "Kinetics and Reaction Mechanism of Transition Metal Complexes", 2nd Revised Ed., VCH, New York.	**1991**
3.	Mukherjee, G.N. and Das, A., "Elements of Bioinorganic Chemistry", Ist Ed., U.N. Dhur & Sons Pvt. Ltd., Calcutta.	**1993**
4.	Gillman, G., "Pharmacological, Basis of Therapeutic", 9th Ed., McGraw Hill.	**1996**
5.	Bertini, I., Gray, H.B., Lippard, S.J. and Valentine, J.S., "Bioinorganic Chemistry", University Science Books, U.S.A.	**1994**
6.	Lippard, S.J. and Berg, J., "Principles of Bioinorganic Chemistry", University Science Books, U.S.A.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-611** Course Title: **Solid-State Chemistry and its Applications**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**
4. Relative weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** **7**. Subject Area: P**EC**
8. Pre-requisite: Knowledge of inorganic chemistry.
9. Objective of Course: To familiarize the students with crystal structures of common inorganic compounds and their characterization methods.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Crystal structure of inorganic compounds:** Overview of close packing, packing efficiency, interstitial sites, limiting radius ratios, method of determination of ionic radii. Ionic crystals containing two or three different elements– FeO, ZnO, CdS, fluorite, antifluorite, nickel-arsenide, CaC_2, CdI_2 and TiO_2, $FeTiO_3$, $MgAl_2O_4$, Fe_2NiO_4, garnets, $BaTiO_3$ and $KNiF_3$. Non-ionic crystals– SiC, (BN)x, giant molecules, layer structures, crystals composed of discrete molecules.	**11**
2.	**Defect structures:** Thermodynamic defects and their consequences, solid electrolytes, non-stoichiometric compounds, F-centers and applications of defects in non-stoichiometric compounds.	**3**
3.	**Methods to synthesize solid-state materials:** Ceramic method, solid-state reaction and its kinetics, hydrothermal, sol-gel, co-precipitation (precursor), vapour phase transport methods. Different methods to grow single crystals.	**6**
4.	**Amorphous inorganic materials:** Glasses, refractories, materials obtained from organometallic chemical vapour deposition (MOCVD). **New materials:** Conducting polymers, carbon nanotubes, carbon nanorods and fullerenes. **Electronic materials:** Insulating, semiconducting and superconducting materials, ferroelectrics and dielectrics.	**6**
5.	**Intercalation chemistry:** Introduction, intercalation reactions in graphite, layered double hydroxides, layered sulfides, applications of intercalation chemistry.	**3**
6.	**Mesoporous materials and their catalytic applications:** Various types of mesoporous materials (oxides, sulphides), tailoring of pore size, applications of mesoporous materials in heterogeneous catalysis.	**3**
7.	**Structural characterization of metal complexes by physical methods:** Extended X-ray absorption spectroscopic (EXAFS), X-ray photoelectron spectroscopic (XPS), X-ray absorption near edge spectroscopic (XANES), electron spin spectrometric (ESR), electron spectroscopy for chemical analysis (ESCA) studies, soild state NMR, HMBC, HMQC, Mössbauer spectroscopic studies of metal complexes, thermal methods (TG, DTA and DSC), atomic force microscopy (AFM) and transmission electron microscopy (TEM).	**10**
	Total	**42**

11. Suggested books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Douglas, B.E., McDaniel, D.H. and Alexander, J.J., "Concepts and Models of Inorganic Chemistry", 3rd Ed., John Wiley & Sons, Inc., New York.	**2001**
2.	West, A.R., "Solid State Chemistry and its Applications", Reprint, Wiley India.	**2013**
3.	Smart, L. and Moore, E., "Solid State Chemistry: An Introduction", Nelson Thornes Ltd.	**2001**
4.	Rao, C.N.R. and Gopalakrishnan, J. "New Directions in Solid State Chemistry", 2nd Ed., Cambridge University Press, Cambridge.	**1997**
5.	Whittingham, M.S. and Jacobson, A.J. (Ed.), "Intercalation Chemistry", Academic Press, New York.	**1982**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-613** Course Title: **Frontiers in Bioinorganic Chemistry**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs): **Theory: 3 Practical: 0**
4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: P**EC**
8. Pre-requisite: Nil
9. Objective of Course: To impart knowledge about metalloproteins from cellular and molecular biological point of view.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Homeostatic mechanism:** Cellular components and pathways in the context of metal ions, homeostatic mechanism in cell – prokaryotes to eukaryotes to human. Evolutionary pathway metals, metallocofactors and prosthetic groups.	**3**
2.	**Metal ion transport and assembly of metalloproteins:** Details of the metal transport in Yeast and in higher organisms, Proteins involved in uptake and efflux, metallochaperones, transcription factors (Ace1 and Mac1, copper sensor). Assembly of metals in protein, photoactivation. Heme synthesis, covalent and non-covalent interactions of heme with protein, assembly of heme in heme proteins-cytochrome c vs cytochrome b5, heme chaperoning and role of CCME. Identification of a protein as heme protein, heme oxygenase, reconstitution of hemeproteins with modified heme/other cofactors and their application in biocatalysis and electron transfer.	**6**
3.	**Molybdenum and tungsten in biology:** Hyperthermophilic and thermophilic bacteria. Mo and W containing enzymes, mechanism of catalytic activity– nitrogenase, sulfite oxidase, nitrate reductase, acetylene hydratase, xanthine oxidase, DMSO reductase. Structural and functional modeling of Mo and W sites and their applications as biocatalysis.	**6**
4.	**Iron in biosystem:** Non-Heme– iron-sulphur proteins, other non-heme iron proteins– lipoxygenase and its implication in cancer research, nitrile hydratase and its application to industry. Structural and functional modeling of heme and non-heme metal-sites and their applications as biochemistry and biocatalysis with examples such as nitrile hydratase, lipoxygenase, acetyl coenzyme synthetase (ACS), DAP1. Heme– catalytic mechanism of nitric oxide synthease and heme oxygenase.	**5**
5.	**Metal ions and diseases:** Role in Alzheimer's disease– Aggregation of proteins, role of copper, zinc and iron. Application of radiochemistry for the identification of metal ions. Metal binding in prion protein–binding of copper and manganese. Manganism– occupational exposure, manganese toxicity, effect on calcium channel, proteomics of manganese toxicity. Inorganic NO-donor and their applications.	**8**
6.	**Bioinformatics and postgenomic era:** Search of metalloprotein and metal binding	

	motif (eg Dap1). De novo design of proteins, artificial heme binding protein, target protein. Modeling with protein structure from protein data bank. DNA intercalation and electron transfer through DNA, RNA metal interactions.	**5**
7.	**Biomineralization:** Biomineralization in the context of bone, teeth and mollusk cells, application into materials science and biomimetic engineering. Bioorganometallic chemistry– introduction and applications.	**4**
8.	**NMR structural biology and structure solution of metalloproteins:** Selection of a target protein, plasmid preparation and overexpression, reparation of sample for NMR. Overexpression of heme protein–cytochrome c vs cytochrome b**.** Labeling of protein by ^{15}N and ^{13}C, standardization of overexpression and purification (heme as well as nonheme). Details of the NMR Experiments for spectral analysis, paramagnetic NMR, structure solution.	**5**
	Total	**42**

11. Suggested books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Cotton, F.A. and Wilkinson, G. "Advanced Inorganic Chemistry", 4th Ed. John Wiley & Sons, New York.	**1980**
2.	Huheey, J.E., Keiter, E.A. and Keiter, R.L. "Inorganic Chemistry: Principles of Structures and Reactivity", 4th Ed., Low Print Edition, Pearson Education Ltd, Asia, Reprint in India.	**2001**
3.	Bertini, I., Gray, H.B. Lippard, S.J. and Valentine, J.S. "Bioinorganic Chemistry", University Science Book, South Asian Edition Reprint.	**2004**
4.	Pecoraro, V.L. "Manganese Redox Enzymes", VCH: New York.	**1992**
5.	Bertini, I., Sigel, A. and Sigel, H. "Handbook on Metalloproteins", Marcel Dekker.	**2001**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OD DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-615** Course Title: **Crystal and Molecular Structure**
2. Contact Hours: **L: 2 T: 0 P: 2/2**
3. Examination Duration (Hrs): **Theory: 2 Practical: 0**
4. Relative weightage: **CWS: 20 PRS: 20 MTE: 20 ETE: 40 PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Nil
9. Objective of Course: To highlight relationship between crystal symmetry and their molecular structure determination process.
10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Symmetry and space group:** Concept of crystal morphology and crystal symmetry, introduction of screw axis and glide plane, crystal systems and space groups, relation between systematic absence and space group.	**6**
2.	**Single crystal X-ray diffraction:** X-ray source, generation of monochromatic wavelength, X-ray diffraction, Bragg equation, concept of reciprocal lattice, Bragg's law in reciprocal lattice, atomic scattering factor, structure factor equation and limiting conditions, intensity and intensity statistics, polarization and Lorentz correction, temperature factor and anisotropic effect, optical classification of crystals, phase problem. Small angle X-ray scattering/diffraction.	**10**
3.	**Single crystal X-ray data handling:** Fourier techniques for electron density calculation in X-ray structure, electron density map, heavy atom method, Patterson function, direct method, normalized structure factor, Σ_2 relationship, least square refinement, anomalous dispersion, twinning in crystal.	**8**
4.	**Neutron diffraction:** Introduction to neutron diffraction, neutron sources and detection of neutrons, scattering cross sections, application to the studies of molecular structure especially for the detection of neighbouring and light atoms.	**4**
	Total	**28**

List of Experiments:

1.	Introduction to the WinGX software to handling single crystal data.
2.	Determination of space group from the *hkl* data set by systematic absences.
3.	Structure solving with isotropic displacement parameter*.
4.	Structure solving with anisotropic displacement parameter and temperature effect.
5.	Treatment of hydrogen for complete structure determination.
6.	Generation of cif, ortep and checking of cif

* This experiment requires two terns.

11. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication/ Reprint
1.	Stout, G.H. and Jensen, L.H., "X-Ray Structure Determination: A Practical Guide", 2nd Ed., John Wiley and Sons, New York.	**1989**
2.	Clegg, W., Blake, A.J., Gould, R.O. and Main, P. "Crystal Structure Analysis: Principles and Practice", Oxford Science Publications.	**2006**
3.	Ladd, M. and Palmer, R. "Structure Determination by X-ray Crystallography", 4th Ed., Kluwer Academic/Plenium Publishers.	**2003**
4.	Massa, W. "Crystal Structure Determination" Springer-Verlag, Berlin, Heidelberg.	**2004**
5.	Buerjer, M.J. "Crystal Structure Analysis", John Wiley and Sons, New York.	**1987**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-617** Course Title: **Supramolecular Chemistry**

2. Contact Hours: **L: 3 T: 0 P: 0**

3. Examination Duration (Hrs): **Theory: 3 Practical: 0**

4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester: A**utumn** 7. Subject Area: **PEC**

8. Pre-requisite: Basic chemistry and spectroscopy.

9. Objective of Course: To impart in depth knowledge of non-covalent interactions in supramolecular systems and their applications.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Fundamentals of supramolecular chemistry:** Definitions, brief overview and examples; types of non-covalent interactions (H-bonding, electrostatic (ion-ion, ion-dipole, dipole-dipole), hydrophobic and steric, π-π, van der Waals), concepts of host-guest complexation with examples from ionophore chemistry, complexation of ions, molecular baskets, chalices and cages– podands, crown ethers, cryptands, calixarenes, macrocyclic effect, complexation of neutral molecules, self-assembly, molecular boxes and capsules, self-complementary species and self-replication.	**8**
2	**Supramolecular chemistry and biological processes:** Cation binding (biological relevance, affinity and selectivity, artificial ionophores, natural and artificial cation channels). Anion and neutral molecule binding –relevance factors affecting affinity and selectivity, anion and neutral molecule binding in biology, artificial hosts for anions, katapinands, guanidinium receptors, receptors based upon Lewis acid-base concepts, enantio-selective anion recognition, cyclodextrins, anion binding based upon ion-dipole interactions, simultaneous anion-cation binding, neutral molecule recognition and binding.	**8**
3	**Synthesis of supramolecules:** Synthesis of macrocycles, synthesis of receptors for cations anions, and neutral molecules, non-covalent synthesis, metal directed self-assembly of complex supramolecular architecture– rotaxanes, catenanes.	**6**
4.	**Physical methods in supramolecular chemistry:** Spectroscopy in supramolecular chemistry, determination of stoichiometry, stability constants, and geometry of complexes, binding constant determination, dynamics of supramolecular systems (solid state *vs* solution behavior).	**8**
5.	**Application of supramolecular chemistry:** Supramolecules in catalysis, as membrane transport, sensors, phase-transfer catalysts, supramolecular devices and switches, memories, logic gates and related systems, molecular scale machines (mechanical rotors, gears and brakes), conversion of light into fuels and light into electricity.	**12**
	Total	**42**

11. Suggested Books:

S.No.	Name of Authors/ Bokks/ Publishers	Year of

		Publication/ Reprint
1.	Steed, J.W. and Aswood, J.L., "Supramolecular Chemistry", Wiley.	**2000**
2.	Dodziuk,,H., "Introduction to Supramolecular Chemistry", Springer, ISBN 1402002149.	**2001**
3.	Beer, P.D., Gale, P.A. and Smith, D.K., "Supramolecular Chemistry", Oxford Chemistry Printers, ISBN-10: 0-19-850447-0.	**1999**
4.	Cragg, P., "A Practical Guide to Supramolecular Chemistry", Wiley-VCH, ISBN: 0-470-86654-3.	**2005**
5.	Schneider, H.J. and Yatsimirsky, A., "Principles and Methods in Supramolecular Chemistry", Wiley-VCH, ISBN: 0-471-97253-3.	**2000**

It has been passed by Senate and there is no change in course contents except the course no. and objectives of the course have been changed.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-619** Course Title: **Modern Organic Synthetic Methods**

2. Contact Hours: **L: 3 T: 0 P: 0**

3. Examination Duration (Hrs): **Theory: 3 Practical: 0**

4. Relative weightage**: CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**

8. Pre-requisite: Basic organic chemistry.

9. Objective of Course: To impart the knowledge of modern synthetic methods used in functional group transformations.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Oxidations:** Oxidations of hydrocarbons (alkanes, alkenes and aromatic), alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, alkenes to diols (Manganese, Osmium-based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based-ozonolysis), alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation), ketones to α-hydroxy ketones, α,β-unsaturated ketones, ester/lactones (Baeyer-Villiger), alcohols to carbonyls (chromium, manganese, aluminum, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents), alcohols to acids or esters, phenols (Fremy's salt, silver carbonate).	**12**
3.	**Named reactions:** Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Brook rearrangement and Tebbe olefination.	**6**
4.	**Protection and deprotection of functional groups:** Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds, chemo- and regioselective protection and deprotection, illustration of protection and deprotection in multi-step synthesis.	**6**
5.	**Retrosynthetic analysis:** Basic principles and terminology of retrosynthesis, guidelines, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions, reversal of polarity (umpolung).	**8**
	Total	**42**

11. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication / Reprint
1.	Carey, F. A. and Sundberg, R. J., "Advanced Organic Chemistry, Part B: Reactions and Synthesis", 5th Ed., Springer.	**2007**
2.	Carruthers, W. and Coldham, I., "Modern Methods of Organic Synthesis", 4th Ed., Oxford University Press.	**2004**
3.	Smith, M.B., "Organic Synthesis", 3rd Ed., Academic Press.	**2010**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-621** Course Title: **Organic Structure Determination**

2. Contact Hours: **L: 3 T: 0 P: 0**

3. Examination Duration (Hrs): **Theory: 3 Practical: 0**

4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**

8. Pre-requisite: Basic organic chemistry.

9. Objective of Course: To familiarize the students with the organic structure determination methods involving spectroscopy.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Electronic spectroscopy:** Electronic transitions in organic molecules, Woodward-Fieser rules for alkenes, Woodward rules for enones, aromatic compounds.	**4**
2.	**Infrared and Raman spectroscopy:** For simple organic molecules, predicting number of active modes of vibrations, analysis of representative spectra of compounds with various functional groups, application of isotopic substitution.	**4**
3.	**Mass spectrometry:** Basic principles, hard and soft ionization techniques, mass analyzer in ESI-MS and MALDI-MS, high resolution MS, isotope abundance, molecular ion, fragmentation processes (McL) of organic molecules, deduction of structure through mass spectral fragmentation.	**6**
4.	**Nuclear magnetic resonance:** Effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant *J*, first order and second order spectra, examples of AB, AX, ABX, AMX and AA′BB′ systems, simplification of second order spectrum, selective decoupling, double resonance, use of chemical shift reagents for stereochemical assignments, ^{13}C NMR, T_1 relaxation, NOE effects, DEPT, determination of number of attached hydrogens, ^{1}H and ^{13}C chemical shifts to structure correlations, study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (fullvalene and related systems). Multinuclear NMR, COSY, DQF-COSY, HETCOR, HMQC, HMBC, TOCSY, ROESY, VGSE.	**20**
5.	**Spectroscopic application**: Structure elucidation of organic compounds using spectroscopic methods.	**8**
	Total	**42**

2. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication / Reprint
1.	Silverstein, R. M., Webseter, F. X. and Kiemle, D., "Spectrometric Identification of Organic Compounds", 7th Ed., John Wiley & Sons.	**2005**
2.	Kemp, W. L., "Organic Spectroscopy", Palgrave.	**2008**
3.	Pavia, D. L., "Spectroscopy", 4th Ed., Cengage.	**2012**
4.	Williams, D. and Fleming, I., "Spectroscopic Methods in Organic Chemistry", 6th Ed., McGraw Hill Education (India) Private Limited.	**2011**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-623** Course Title: **Organic Semiconductors**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**

4. Relative weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits: **3** 6. Semester: **Autumn** **7**. Subject Area: P**EC**

8. Pre-requisite: Basic organic chemistry and spectroscopy.

9. Objective of Course: The course will deal with rapidly emerging areas in organic electronic materials.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Introduction:** General description of conjugated organic oligomers, dendrimers and polymers. Conjugated polymer structural types (polyacetylenes, polyphenylene-vinylenes, polyphenyeleneethynylenes, polyfluorenes, polythiophenes, poly-phenylenes, polyanilines, water soluble polymers, phosphorescent polymers). Carbon-rich compounds, Cross-conjugation.	**6**
2	**Synthesis:** Useful synthetic methods for the construction of conjugated organic oligomers and polymers. C-C and C-heteroatom coupling reactions – historical context and latest developments. Representative examples. Mechanistic consideration. All-benzenoid polycyclic aromatic hydrocarbons– synthesis, self-assembly and applications in organic electronics. Solid state strategy for the preparation of carbon-rich polymers.	**10**
3	**Properties:** Electronic structure of organic semiconductors – relationship between two view points: solid state physics and molecular picture of conjugated organics. Electrochemistry, electrochromism and energy level measurements. Charge transport (electronic conduction in photoactive molecular-wires). Luminescence. Energy transfer and electron transfer. Excitation dynamics in organic semiconductors. Fluorescence sensing. Non-linear optical properties.	**14**
4.	**Applications:** Field-effect transistors, light-emitting diodes, photovoltaics and solar cells–device architectures, materials, characterization and theory of operation. Biosensors – electrochemical detection, fluorescence optical amplification (protein, DNA and RNA sensing), solid state applications (DNA chips and micro arrays).	**12**
	Total	**42**

11. Suggested books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Haley, M.M. and Tykwinski, R.R. (Ed.), "Carbon-Rich Compounds: From Molecules to Materials" Wiley.	**2006**
2.	Singh, J., "Smart Electronic Materials: Fundamentals and Applications", Cambridge University Press.	**2005**
3.	Fraxedas, J., "Molecular Organic Materials: From Molecules to Crystalline	**2006**

	Solids", Cambridge University Press.	
4.	Schubert, E.F., "Light-Emitting Diodes", 2nd Ed., Cambridge University Press.	**2006**
5.	Brabec, C., Dyakonov, V., Parisi, J. and Sariciftci, N.S. (Ed.), "Organic Photovoltaics", Springer.	**2003**
6.	Agranovich, V.M. (Ed.), "Organic Nanostructures", IOS press.	**2002**
7.	Norio, M. (Ed.), "Cross-Coupling Reactions: A Practical Guide", Springer.	**2002**

This has been passed by Senate and no change in course contents except course no. has been changed.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN -625** Course Title: **Proteins and Polypeptides**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs): **Theory: 3 Practical: 0**
4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Basic knowledge of analytical techniques.
9. Objective of Course: To provide advanced knowledge in protein chemistry.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Proteins and peptides:** General nature, characteristics, introduction to primary, secondary and tertiary structures.	**4**
2.	**Separation and purification methods:** Electrophoresis, isoelectric focussion, gel filtration, affinity chromatography, and ion exchange – choice of gel support materials (agarose, cellulose, polyacrylamide, glass beads, DEAE-cellulose, CM-cellulose etc.) HPLC.	**8**
3.	**Fragmentation of polypeptides:** Chemical methods – cleavage of di-sulfide bonds, oxidation, partial acid hydrolysis, cleavages at methionine, tryptophan, tyrosine, cysteine. Enzymic methods – protein modification reactions disulphide bond cleavage, alkylaton of sulphydryl groups, modification of lysine and arginine residues. Specificity and conditions for trypsin, thrombin, chymotrypsin, thermolysin, pepsin papaine.	**12**
4.	**Determination of peptide sequences:** Manual sequencing, solid phase sequence analysis, automated liquid phase sequence analysis, microsequence analysis using a gas-liquid solid-phase sequenator, C-terminal sequence analysis.	**6**
5.	**Applications of electron impact mass spectrometry,** X-ray crystallography and electron microscopy**:** In the structural analysis of peptides and proteins.	**6**
6.	**Peptide mapping and peptide synthesis**: Prediction of peptide and protein structure. Peptide synthesis including solid-phase and automated synthesizers.	**6**
	Total	**42**

11. Suggested books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Lehninger A.L., "Biochemistry", North Publishers.	**1980**
2.	Stryer L., "Biochemistry", CBS Publications and distributors.	**1981**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN- 627** Course Title: **Advanced Surface and Colloidal Chemistry**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs): **Theory: 3 Practical: 0**
4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Knowledge of physical chemistry.
9. Objective of Course: To impart advanced knowledge of surface and interfacial phenomenon.
10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Surfactants and Interfacial Phenomena:** Classification, micellization, c.m.c. and its determination. Shape and structure of micelles, effect of additives on micellization, thermodynamics of micellization, solubilization and applications, effect of electrolytes on solubilization. Macro and micro emulsions, dispersion and aggregation of solids by surfactants.	**9**
2.	**Membranes and their Applications:** Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.	**6**
3.	**Adsorption on solids and porous materials:** Model for multilayer adsorption, BET isotherm and application to different types of adsorbents, adsorption by porous, non-porous and microporous solids. Estimation of specific surface area and pore size distribution. Special problems encountered with very narrow pore size material and adsorption from liquid phase.	**7**
4.	**Colloid systems and their properties:** Origin of the charges, electro-kinetic phenomena, electrophoresis, electroosmosis, sedimentation and streaming potential. The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids. Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates. Organic and inorganic gels and clay colloids.	**8**
5.	**Macromolecules:** Concepts of mass and number average molecular weights, methods of determining molecular weights (osmometry, viscometry, diffusion and light scattering method), sedimentation, fractional properties of macromolecules, statistical distribution of end to end dimension, calculation of average dimension of various chain structures.	**12**
	Total	**42**

11. Suggested books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Hunter, R. J., "Foundation of Colloid Science", Oxford Univ. Press.	**2009**
2.	Lyklema, J., "Fundamentals of Interface and Colloid Science", Academic Press San Diego.	**2000**

3.	Adamson, A.W.,"Physical Chemistry of Surfaces", 5th Ed., John Wiley and Sons, New York.	**1990**
4.	Kruyt, H.R., "Colloid Chemistry" Vol. I & II. Elsevier Press.	**1991**
5.	Greg, S.J. and Singh, K.S.W., "Adsorption, Surface Area and Porosity", 2nd Ed., Academic Press. U K.	**1982**
6.	Flory P. J., "Principles of Polymer Chemistry", 1st Ed., Cornell University Press.	**1953**
7.	Rubinstein M. and Colby R. C., "Polymer Physics", 1st Ed., Oxford University Press.	**2003**
8.	Billmeyer, F. W., "Textbook of Polymer Science", 3rd Ed., Wiley India Private Limited	**2007**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-629** Course Title: **Advanced Physical Chemistry**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) Theory **03** Practical **0**
4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: Knowledge of physical chemistry
9. Objective of Course: To familiarize the students with advanced kinetics, thermodynamics and quantum chemistry.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Advanced chemical kinetics:** Theories of unimolecular reactions, kinetics-proton transfer and electron transfer reactions, fast reactions–rapid flow, stopped-flow and relaxation techniques, molecular beam method, diffusion controlled reactions, oscillatory reactions, linear free energy relationship, elucidation of mechanism from kinetic data.	**14**
2.	**Statistical mechanics and irreversible thermodynamics:** Phase space, Liouville's theorem, Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac statistics. Affinities and fluxes, reversible and irreversible processes, entropy production for some important irreversible processes, entropy flow due to exchange of mater and energy, entropy changes due to chemical reaction, affinity and coupling of chemical reaction, the phenomenological laws and equations and their applications in chemistry, fluctuations, response functions, time correlation function, distribution function.	**14**
3.	**Advanced quantum chemistry:** Dirac Bra-ket notation, addition of angular momentum, use of ladder operators– rigid rotor and harmonic oscillator, variation method– treatment of He atom, perturbation method– examples of anharmonic oscillator, He atom, Stark and Zeeman splitting, Hartree-Fock method, introduction to post Hartree-Fock methods.	**14**
	Total	**42**

11. Suggested books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	Laidler, K.J., "Reaction Kinetics", Anand Sons, New Delhi.	**2005**
2.	Kondepudi, D. and Prigogine, I. , "Modern Thermodynamics: From Heat Engines to Dissipative Structures", John Wiley & Sons.	**1998**
3.	Callen, H. B., "Thermodynamics and an Introduction to Thermostatistics", John Wiley and Sons.	**1985**
4.	Bransden, B.H. and Joachain, C.J., "Quantum Mechanics", Addison-Wesley.	**2000**
5.	Sakurai, J. J., "Modern Quantum Mechanics", Pearson Education.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN- 631** Course Title: **Materials Chemistry**

2. Contact Hours: **L: 2** **T: 0** **P: 2/2**

3. Examination Duration (Hrs): **Theory: 2** **Practical: 0**

4. Relative Weightage**:** **CWS: 20** **PRS: 20** **MTE: 20** **ETE: 40** **PRE: 0**

5. Credits: **3** 6. Semester**: Autumn** 7. Subject Area**: PEC**

8. Pre-requisite: Structure, Bonding and Properties of Solids.

9. Objective: To introduce the students in the area of materials chemistry.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Reactions in the solid state and phase transitions:** General principles, kinetics of solid-state reactions-nucleation and diffusion rate, Wagner mechanism, Kirkendall effect, Vegard's law, phase transition-Ehrenfest classification and Lanbda transition, structural and magnetic phase transitions order-disorder, martensitic and atensitic, ferro-para.	**4**
2.	**Structure determination**: X-ray powder diffraction - lattice refinement, pattern simulation, refinement of crystal structure– Rietveld method, profile fitting, refinement of occupancy and thermal factors, isotropic and anisotropic displacements, reliability factors. Neutron scattering–elastic and inelastic, diffraction experiments with neutron, chemical and magnetic structure, magnetic scattering, elucidation of magnetically ordered structures.	**8**
3.	**Advanced materials and devices:** Magnetic materials, dilute magnetic semiconductors, magnetic shape-memory alloys, magnetoresistive, semiconducting, superconducting, multiferroic and spintronic materials, graphene and its nanocomposites, Li-ion batteries, solid oxide fuel cells, perovskite solar cells, magnetic tunnel junctions and spin-valves.	**10**
4.	**Preparation methods and processing of materials:** Revisit to general synthetic routes- gas-solid, liquid-solid and solid-solid methods. Sputtering, pulsed laser deposition (PLD), molecular beam epitaxy (MBE), liquid quenching, arc melting, induction, zone melting, chimie-douce, high-pressure, mechanochemical, ball-milling methods.	**6**
	Total	**28**

List of experiments:

1.	Drawing and visualization of crystal structures and structural parameter analysis.
2.	Indexing of powder X-ray diffraction (PXD) patterns.
3.	Lattice parameter refinement and doping analysis.
4.	Simulation of PXD patterns and occupancy modelling in doped systems.
5.	Whole pattern fitting-Le Bail method.
6.	Rietveld refinement of PXD data for crystal structure determination.

7. 8. 9.	Density functional theory softwares. Electronic structure calculation of metals/insulators. Electron localization function and Fermi surface calculation.

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1.	West, A. R., "Solid State Chemistry and its Applications", Reprint, Wiley India.	**2013**
2.	Rao, C.N.R. and Gopalakrishnan, J., **"**New Directions in Solid State Chemistry", 2nd edn., Cambridge University Press.	**1997**
3.	Stout, G.H. and Jensen, L.H., "X-Ray Structure Determination: A Practical Guide", 2nd edn., Wiley-Interscience.	**1989**
4.	Giacovazzo, C., Artioli, G., Monaco, H. L., "Fundamentals of Crystallography", Oxford University Press.	**2006**
5.	"Magnetic Materials: Fundamentals and Device Applications", Nicola Spaldin, Cambridge University Press.	**2003**
6.	"Electronic Structure of Materials", A. P. Sutton, A. D. Sutton, Oxford University Press.	**1993**

Sl. No.	Softwares and Databases		Source
1.	Diamond	(commercial)	www.crystalimpact.com
2.	XCrysden	(freeware)	http://www.xcrysden.org/
3.	ICSD	(commercial)	www.fiz-karlsruhe.com
4.	Powder Cell	(freeware)	www.ccp14.ac.uk
5.	FullProf	(freeware)	www.ill.eu
6.	Full Potential Localized Orbital (FPLO) Code	(commercial)	www.fplo.de

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: DEPARTMENT OF CHEMISTRY

1. Subject Code: **CYN-633** Course Title: **Nanoscale Materials: Properties and Applications**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs): **Theory: 3** **Practical: 0**

4. Relative Weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PEC**

8. Pre-requisite: Nil

9. Objective: To impart fundamental understanding on nanoscale materials, their properties and applications.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Introduction to nanoscale materials:** The nano-length scale, quantum confinement effect, consequences of quantum confinement of electrons, conceptual development of band theory – from molecules to clusters/quantum dots to macroscopic crystals, material dependence of nanoscale and quantum size-effect, consequences of carrier confinement in semiconductors and metals.	**6**
2.	**Structure of nanomaterials:** Crystalline and amorphous nanomaterials, nanocrystals, surface energy and crystal facets, equilibrium shape of nanocrystals, Wulff construction, Roughening temperature, surface energy as a function of surface curvature, chemical potential and solubility as a function of surface curvature and particle size, Ostwald ripening, nucleation and growth of nanoparticles.	**6**
3.	**Physical and chemical characteristics of nanomaterials:** Surface area measurement, determination of size and textural studies, composition and elemental analysis, high chemical reactivity of nanoscale materials, effect of size and shape on nanocrystal reactivity, agglomeration and sintering of nanomaterials, dispersibility and chemical stability of nanoparticles in solution, surface modification of metallic and semiconductor nanoparticles, nanofabrication and nanomanipulation	**12**
4.	**Synthesis and applications of nanomaterials:** Concepts of top-down and bottom-up approaches, chemical, aerogel, aerosol, spray-pyrolysis, microemulsion, solvothermal, sonochemical, and microwave methods of synthesis. Reactivity studies by adsorption–SO_2, CO_2, H_2S, CCl_4 and chemical warfare agents, destructive adsorption, detoxification by adsorption, air purification, desulphurization, biocidal applications, modification of nanocrystalline metal oxides and their applications.	**14**
5.	**Toxicology of nanomaterials:** Health concerns of using nanomaterials, inhalation toxicity, oral toxicity, environmental toxicity, cyto- and bio-toxicity of	**4**

	nanomaterials, environmental protection, precautions and case studies.	
	Total	**42**

11. Suggested Books:

Sl. No.	**Name of Authors/ Books/ Publishers**	**Year of Publication/ Reprint**
1.	Klabunde, K.J. (Ed.), "Nanoscale Materials in Chemistry", Wiley-Interscience, New York.	**2001**
2.	Schmid, G. (Ed.), Nanoparticles: From Theory to Application", Wiley-VCH, Weinheim.	**2004**
3.	Cao, G. and Wang, Y., "Nanostructures and Nanomaterials: Synthesis, Properties and Applications", 2nd Revised Ed., World Scientific.	**2011**
4.	Rodriguez, J. A. And Fernandez-Garcia, M. (Ed.), "Synthesis, Properties and Applications of Oxide Nanomaterials", John Wiley, New York.	**2006**
5.	Rao, C.N.R., Müller, A. and Cheetham, A.K., "The Chemistry of Nanomaterials: Synthesis, Properties and Applications", Vol. 1 and 2, Wiley-VCH Verlag, Weinheim.	**2004**
6.	West, A. R. "Solid State Chemistry and its Applications", Reprint, Wiley India.	**2013**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-635** Course Title: **Advanced Magnetic Resonance Spectroscopy**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**

4. Relative Weightage**: CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PEC**

8. Pre-requisite**:** Basic knowledge of magnetic resonance spectroscopy**.**

9. Objective: To provide advance knowledge of NMR and ESR techniques for structure elucidation of molecules and radicals.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Magnetic resonance:** Nuclear spin, Zeeman effect, Larmour precession, Boltzmann distribution of spin population, magnetic field and resolution, folded signals , peak broadening and solid state effect.	**3**
2.	**Relaxation processes:** Longitudinal and cross sectional relaxation mechanism of magnetic vector, Bloch equation, pulse strength and magnetization vector, spin-saturation, spin-inversion and spin-echo methods for relaxation times. Effect of chemical shift anisotropy, scalar coupling, dipole-dipole coupling and electron interactions on relaxation time.	**4**
3.	**Chemical shift:** Shielding coefficient and chemical shift, low field and high field chemical shift, solvent effect and factors influencing the chemical shift. anisotropic effect in benzene and carbonyl compounds, chemical and magnetic equivalence.	**3**
4.	**Scalar and dipolar couplings:** Coupling of nuclear spins, coupled spins energy diagrams and sign of coupling constant in AX and AB systems. Geminal and vicinal coupling and Karplus relation for tetrahedral angle. Dipolar couplings in solids and bond length.	**3**
5.	**Double resonance:** Double resonance and Simplification spectra, pulse sequence, spin polarization transfer and Nuclear Overhauser effect, progressive and retrogressive internuclear relationship , selective decoupling, J-modulated spin-echo and attached proton test (APT), insensitive nuclei enhancement by polarization transfer (INEPT) and distortion less enhancement by polarization transfer (DEPT). Fourier transform and ^{13}C NMR spectroscopy.	**6**
6.	**Dynamic NMR:** Chemical and dynamic processes by NMR, temperature dependant rotamers and colescence temperature. Dynamic equilibrium, line shape and Gibb's free energy.	**4**
7.	**2-Dimensional NMR spectroscopy:** Basics of two dimensional NMR spectroscopy, 2D correlation (COSEY) and 2D Nuclear Overhauser enhancements Spectroscopy (NOESY) experiments and their applications in structural elucidation of organic molecules.	**8**
8.	**ESR spectroscopy:** Electron spin and magnetic moment, g-factor, triplet state and spin transitions, hyperfine structures, Zerofield splitting, Kramer degeneracy and	**5**

	double resonance.	
9.	**NQR spectroscopy:** Nuclear quadrupole moment and electrical field gradient, quardrupole coupling constants (NQCC) and asymmetry parameter (□), pure NQR and Zeeman spectra of spin 1 and spin 3/2 systems, the Towners-Dailey theory and interpretation of NQCC in terms of characteristic of the bonds and effects of other parameters.	**6**
	Total	**42**

11. Suggested Books:

S. No.	**Name of Authors/ Books/ Publishers**	**Year of Publication/ Reprint**
1.	Gunther, H., "NMR Spectroscopy. Basic Principles, Concepts and Applications in Chemistry", Wiley India.	**2010**
2.	Banwell, C.N. and McCash, M. , "Fundamentals of Molecular Spectroscopy", McGraw Hill Education Pvt. Ltd, India.	**2013**
3.	Graybeal, J.D., "Molecular Spectroscopy", McGraw-Hill Book Company, India.	**1988**
4.	Drago, R.S., "Physical Methods in Inorganic Chemistry", Affiliated East West Press , Pvt. Ltd. India.	**2010**
5.	Weil, J.A., Bolton, J.R. and Wertz, J.E., "Electron Paramagnetic Resonace", Wiley-Interscience, New York.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-606** Course Title: **Total Synthesis**

2. Contact Hours: **L: 3 T: 0 P: 0**

3. Examination Duration (Hrs): **Theory: 03 Practical: 0**

4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**

5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PEC**

8. Pre-requisite: **CYN-506**

9. Objective of Course: To familiarize the students with the tactics and strategies in the total synthesis of targeted compounds.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	Introduction to strategies for synthesis of complex molecular architectures.	**2**
2.	Synthesis of antibiotics – penicillin V and tetracycline.	**7**
3.	Synthesis of alkaloids – reserpine and camptothecin.	**7**
4.	Synthesis of terpenoids – β-pinene, camphor, abietic acid and β-amirine.	**8**
5.	Synthesis of steroids and hormones – cholesterol, progesterone and cortisone.	**8**
6.	Synthesis of prostaglandins PGE_2 and $PGF_{2\alpha}$; glycosidic pigments anthocyanins and quercetin; macrocyclic lactam fluvirucin-B_1-aglycone; and vitamin biotin.	**10**
	Total	**42**

11. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication / Reprint
1.	Finar, I.L., "Organic Chemistry", Vol .2, 5th Ed., ELBS.	**1975**
2.	Corey, E.J. and Cheng, X.-M., "The Logic of Chemical Synthesis", Wiley–VCH, Weinheim.	**1995**
3.	Nicolaou, K.C. and Sorensen, E.J., "Classics in Total Synthesis", Wiley–VCH, Weinheim.	**1996**
4.	Gewert, J.A., Gorlitzer, J., Götze, S., Looft, J, Menningen, P., Nobel, T., Schirock, H. and Wulff, C., "Organic synthesis workbook", Wiley–VCH, Weinheim.	**2000**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OD DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-608** Course Title: **Chemical Biology**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs): **Theory: 3 Practical: 0**
4. Relative weightage: **CWS: 25 PRS: 0 MTE: 25 ETE: 50 PRE: 0**
5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PEC**
8. Pre-requisite: Knowledge of inorganic, organic synthesis and basic of fluorescence.
9. Objective of Course: To develop the knowledge of applying chemical tools in recognition process of biological systems.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Application of spectroscopy in chemical biology:** Brief introduction to chemical biology, biological structures and its constituents, spectroscopic tools to rationalize chemical reactions in biosystems, design of fluorescent and fluorogenic probes and optical biosensor molecules.	**9**
2.	**Chemical reactions suitable for biological applications:** Solid phase peptide synthesis, bioorthogonal reactions, functional group specific ligation techniques, strategies for attachment of synthetic molecules to biomolecules, Staudinger ligation, native chemical ligation, click chemistry, site selective protein modification.	**12**
3.	**Chemical interpretation of protein labeling technologies:** Green fluorescence protein (GFP), fluorescein arsenical hairpin (FlAsH), SNAP tag, CLIP tag, mutant β-lactamase (BL) tag, halo tag, and their selective significant applications.	**12**
4.	**Chemistry behind artificial cellular components:** Synthetic membranes, vesicles – ion transport, unnatural amino acids and their incorporation, DNA chemistry and its uses, nucleic acid templated chemistry, chemistry of morpholino and locked nucleic acid (LNA), siRNA.	**9**
	Total	**42**

10. Suggested books:

S. No.	Authors/Title/Publishers	Year of Publication/ Reprint
1.	Waldmann, H. and Janning, P. "Chemical Biology: Learning Through Case Studies", Wiley-VCH, Weinheim.	**2009**
2.	Dobson, C.M., Gerrard, J.A. and Pratt, A.J. "Foundations of Chemical Biology", Oxford University Press.	**2002**
3.	Miller, A. and Tanner, J. "Essentials Of Chemical Biology: Structure and Dynamics of Biological Macromolecules", Wiley.	**2002**
4.	Waldmann, H. and Janning, P. "Chemical Biology: A Practical Course", Wiley-VCH, Weinheim.	**2004**
5.	Hermanson, G.T. "Bioconjugate Techniques", 3rd Ed., Academic Press.	**2013**

6.	Lackowicz, J.R. "Principles of Fluorescence Spectroscopy", 3rd Ed., Springer.	**2006**
7.	Blackburn, G.M., Gait, M.J., Loakes, D. and Williams, D.M. "Nucleic Acids in Chemistry and Biology", 3rd Ed., RSC Publishing.	**2006**
8.	Schreiber, S.L., Kapoor, T. and Wess, G. "Chemical Biology: From Small Molecules to Systems Biology and Drug Design", Vol. 1-3, Wiley-VCH, Verlag GmbH & Co. KGaA.	**2007**

INDIAN INSTITUTE OF TECHNOLOGY ROOKEE

NAME OD DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-610** Course Title: **Molecular Modeling and Simulations**
2. Contact Hours: **L: 2** **T: 0** **P: 2/2**
3. Examination Duration (Hrs.): **Theory: 2** **Practical: 0**
4. Relative Weightage: **CWS: 20** **PRS: 20** **MTE: 20** **ETE: 40** **PRE: 0**
5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PEC**
8. Pre-requisites: CYN-501 and CYN-503.
9. Objective: To provide knowledge on computational methods in chemistry
10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Fundamentals of electronic structure:** Basis function–hydrogen-like, Slater-type and Gaussian type orbitals, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets, correlation consistent basis sets, basis set super position error, energy minimization methods–derivative and non-derivative methods-simplex method, steepest descents method, Newton-Raphson method, minima, maxima and saddle points.	**8**
2.	**Semi empirical and Ab intio methods:** Approximation methods, self consistent field treatment of polyatomic molecules, closed shell systems –restricted Hartree Fock calculations, open shell systems–ROHF and UHF calculations, The Roothan–Hall equations, Koopman's theorem, HF limit and electron correlation, introduction to post Hartree-Fock and density functional methods.	**8**
3.	**Electronic properties:** Dipole moment, electrostatic potential, frequencies, population analysis, Mulliken and Lowdin analysis, solvent effects, polarizable and nonpolarizable models.	**6**
4.	**Introduction to simulation methods**: Molecular mechanics, Monte carlo and molecular dynamics simulations, periodic boundary conditions, radial distribution function, calculation of thermodynamic properties.	**6**
	Total	**28**

List of practicals:

1. Potential energy curves for covalently bonded molecules and van der Waals complexes.
2. Geometry optimization of molecules at different levels of theory.
3. Frequency calculation of molecules.
4. Excited states of small molecules.
5. Determination of energy barrier for simple reactions.
6. Constructing the distribution function for liquid water using molecular dynamics method.
7. Calculation of specific heat capacities of liquid water at different conditions.

11. Suggested books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication/

		Reprint
1.	Jensen, F., "Introduction to Computational Chemistry", John Wiley & Sons Ltd.	**1999**
2.	Leach, A., "Molecular Modeling: Principles and Applications", Prentice Hall.	**2001**
3.	Cramer, C. J., "Essentials of computational chemistry: Theories and models", John Wiley & Sons.	**2002**
4.	Levine, I. N. "Quantum Chemistry", 7th Ed., PHI Learning Pvt. Ltd., Delhi.	**2013**

INDIAN INSTITUTE OF TECHNOLOGY ROOKEE

NAME OD DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. 1. Subject Code: **CYN-612** Course Title: **Carbon Nanomaterials and their Applications**

2. Contact Hours: **L: 3** **T: 0** **P: 0**

3. Examination Duration (Hrs.): **Theory: 3** **Practical: 0**

4. Relative Weightage: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**

5. Credits: **3** 6. Semester: **Spring** 7. Subject Area: **PEC**

8. Pre requisite: Nil

9. Objective of course: To familiarize the student with applications of carbon nanomaterials.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Introduction and synthetic approaches:** Uncatalysed and catalyzed synthesis of carbon nanomaterials, supported nanomaterials, nanodiamonds, fullerenes, single and multi wall carbon nanotubes, carbon dots, carbon fibre.	**6**
2.	**Biological applications:** Biomedical application of graphene, biosensors based on carbon materials, tissue engineering, fullerenes in photodynamic therapy, interaction of fullerenes with DNA, an overview of application in cancer therapy, environmental impact of carbon materials, toxicological effect on fish, invertibrates, bacteria, soil microbes.	**10**
3.	**Carbon nanomaterials for sensing applications:** Carbon nanotubes and graphene for sensing applications, graphene transistor, single molecule memory devices, organic transistor odour sensor and spintronics.	**8**
4.	**Carbon nanomaterials for electronics, optoelectronics and photovoltaics:** Carbon nanotubes–electronic and optoelectronic applications, transistors for digital electronics, graphene–electronics and optoelectronics, digital electronics, photovoltaics– fullerenes**,** carbon nanotubes, graphene.	**14**
5.	**Space applications:** Polymer and carbon nanotube composites for space applications, meteoroids, micrometeoroids, and space-debris, conductive coatings for electrostatic discharge, thermal conductivity, space elevator, solar sails.	**4**
	Total	**42**

11. Suggested books:

S. No.	Name of Authors/Books/Publishers	Year of Publication/ Reprint
1.	Philip, W. H.-S and Akinwande, D., "Carbon Nanotube and Graphene Device Physics", Cambridge University Press.	**2011**
2.	Reich, S., Thomsen, C. and Maultzsch, J., "Carbon nanotubes: Basic concepts and physical properties", Wiley-VCH.	**2004**
3.	Saito, R., Dresselhaus, G. and Dresselhaus, M. S., "Physical Properties of Carbon Nanotubes", Imperial College Press, London .	**1998**
4.	Challa, K.(Ed.), "Carbon Nanomaterials", Vol. 9., Wiley-VCH.	**2011**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject : **CYN-614** Course Title: **Enantiomeric Separation**

2. Contact Hours: **L: 2** **T: 0** **P: 2/2**

3. Examination Duration (Hrs): **Theory: 2** **Practical: 0**

4. Relative weightage: **CWS: 20** **PRS: 2 0** **MTE: 20** **ETE: 40** **PRE: 0**

5. Credits: **3** 6. Semester: **Spring** 7. Subject Are: **PEC**

8. Pre-requisite: Knowledge of stereochemistry of organic compounds.

9. Objective of Course: To provide knowledge of modern chromatographic separation methods.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Introduction:** Modern stereochemical concepts– chirality and molecular structure, definitions and nomenclature.	**2**
2.	**Techniques used for studies of optically active compounds:** Methods not involving separation– polarimetry, NMR, isotope dilution, calorimetry, enzyme techniques. Determination of absolute configuration– X-ray, ORD, CD and chromatography based on comparison.	**4**
3.	**Modern chromatographic separation methods:** Basic chromatographic theory, instrumentation – gas and liquid chromatography.	**4**
4.	**Direct optical resolution:** Theory, general aspects of chiral recognition models–coordination to transition metals, charge transfer interaction, inclusion phenomena. Thermodynamic and kinetic considerations.	**4**
5.	**Chiral gas chromatography:** Phases based on chiral metal complexes, inclusion effects-relative merits.	**4**
6.	**Chiral liquid chromatography:** CSPs based on naturally occurring and synthetic polymers, bonded synthetic chiral selectors, CMPAs.	**6**
7.	**Analytical applications:** Amino acids, natural products, pharmaceuticals, microbial and enzymatic reactions.	**4**
	Total	**28**

List of Experiments:

1. Isolation of L-asparagine from *Asparagus* or Soybean, its characterization, determination of specific rotation, change of specific rotation from levo to dextro in acidic solution.
2. Isomerization of 2-aryl propionic acid or other simple less expensive optically pure compound(s).
3. Resolution of (±)-mandelic acid.
4. Separation of (-)-ephedrine and (-)-mandelate.
5. TLC enantioseparation of DL-amino acids on plates impregnated with an optically pure base.
6. Ligand exchange TLC enantioseparation of DL-amino acids (or commercial racemic pharmaceuticals) using Cu(II)-L-Pro complex.
7. Enantiomeric separation of (±)-2-butanol via its reaction with (+)-tartaric acid.
8. Racemization studies using (*R*)-3-phenyl-2-butanone or (*S*)-3-methyl cyclohexanone.
9. Synthesis of chiral variant of Sanger's reagent,

11. Suggested books:

S.No.	Name of Authors/ Books/ Publishers	Year of Publication/ Reprint
1	Kowalska,T. and Sherma, J., "Preparative Layer Chromatography", CRC-Taylor & Francis, New York.	**2006**
2	Ahuja, S., "Chromatography and Separation Science", Academic Press, Amsterdam.	**2003**
3	Snyder, L.R., Glajch, J.L., and Kirkland, J.J., "Practical HPLC Method Development", Wiley, New York.	**1988**