INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-511** Course Title: **Quantum Mechanics, Symmetry & 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:

Sl. No.	Contents	Contact Hours
1.	**Quantum Mechanics:** Postulates of Quantum Mechanics, observables, operators, functions, Schrödinger wave equation, hydrogen atom, transformation of coordinates, separation of variables, the Φ equation, the Θ equation, the radial equation, quantum states, the electron spin, energy states of hydrogen atom, wave functions of hydrogen atom, radial distribution curves and angular dependence of wave function, graphical representation of orbitals, multielectron systems, term symbols, introduction to approximation methods.	16
2	**Theories for Chemical Bonding**: Valence bond theory, MO theory and Huckel MO approach	6
3.	**Molecular Symmetry:** Symmetry elements and symmetry operations, symmetry elements and optical isomerism, symmetry point groups, various steps to identify point groups of molecular species and some illustrative examples, classes of symmetry operation.	6
4.	**Group Theory:** Representation of a group, the great orthogonality theorem and its consequences, character tables, representation for cyclic groups, the direct product, reducible and irreducible representations, analysis of reducible representations, reducible representations for molecular motions and its analysis.	8
5.	**Applications of Group Theory:** Group theory and Quantum mechanics, vanishing integrals, orbital overlap, symmetry adapted linear combinations, molecular shapes, symmetry of normal modes of vibrations, prediction of infrared and Raman activity, electronic transitions.	6
	Total	42

11. Suggested Books

Sl. No	Name of Authors/Books/Publisher	Year of Publication/ Reprint
1.	Simons J. and Nichols J., "Quantum Mechanics in Chemistry", Oxford University Press.	1997
2.	Levine I. R., "Quantum Chemistry", Pearson Education, Inc.	2003
3.	Szabo A., and Ostlund N. S. "Modern Quantum Chemistry", Tata McGraw Hill.	1989
4.	Cotton F. A., Chemical Applications of Group Theory", Wiley.	1999

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-512** Course Title: **Organometallic Chemistry**

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**: Spring** 7. Subject Area**: PCC**

8. Pre-requisite**: Nil**

9. Objective: To impart basic and advanced concepts in organometallic chemistry.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Main Group Organometallics:** Introduction, review of comparative aspects of synthetic methods, reactivity and bonding in ionic, covalent, electron deficient and electron rich organometallic compounds.	5
2.	**Important Reactions of Organometallics**: Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands.	4
3.	**Structure and Bonding in Organometallic Compounds:** Introduction, 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 evidence and consequences of bonding.	4
4.	**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.	6
5.	**Transition Metal Organyls with Metal-Carbon Multiple Bonding:** Transition metal-carbenes, -carbynes, -bridging carbenes/carbynes, reactions of carbene/carbyne complexes: ligand substitution, nucleophilic, electrophilic attack, dismutation, ligand coupling reactions.	6
6.	**Organotransition Compounds with Multicenter Bonds (non-classically bonded):** Concept of hapticity, transition metal complexes of alkenes, Ziese salt, allenes, alkynes, allyls, butadienes; cyclic π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cycloheptatrienyls and cyclooctatetraenes; reactions and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxional compounds, bimetallic and cluster complexes.	8
7.	**Applications of Transition Metal-Organic Compounds in Catalysis:** Hydroformylation, hydrogenation of olefins, synthesis of chiral pharmaceuticals, olefins metathesis, Wacker process, polymerization (Zeigler-Natta Catalyst), cyclooligomerisation of acetylene using nickel catalyst (Reppe catalyst), polymer-bound catalysts and importance of organometallic compounds in certain biological systems.	6
8.	**Bioorganometallic Chemistry:** Organometallo-therapeutic drugs, enzyme inhibitors, biological importance of Vitamin B_{12} and coenzymes and their biomimetic studies, bioorganometallic compounds as drugs.	3
	Total	42

11. Suggested Books:

S. No.	Name of Books / Authors	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.	Purcell K.F. and Kotz J.C., "Inorganic Chemistry", Saunders, London,	**1977**
4.	Hill A.F., "Organotransition Chemistry", The Royal Society of Chemistry, Cambridge.	**2002**
5.	Bochmann, M. (Ed.), "Oxford Premier Series on Organometallics", Vol. 1 and 2. Oxford Press.	**2002**
6.	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 DEPT/CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject: **CYN-521** Course Title: **Thermodynamics & Surface Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) Theory **03** Practical **00**
4. Relative Weight: **CWS 25** **PRS 0** **MTE 25** **ETE 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PCC**
8. Pre-requisite: **Nil**
9. Objective of Course: To familiarize students with thermodynamics aspects of chemical and phase equilibria, surface process and ionic systems.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Laws of Thermodynamics:** Third law of thermodynamics, Nernst theorem, attainability of absolute zero, the 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.	**14**
2.	**Statistical Mechanics**: Statistical Method, probability of distribution and ensembles, microcanonical ensemble, entropy and probability, canonical ensemble, Boltzmann distribution, partition function and their evaluation and relation with thermodynamic properties, evaluation of entropy of gasses by statistical method, grand canonical ensemble and other ensembles: partition function	**12**
3.	**Surface Chemistry**: Surface phenomenon, electrical phenomenon of interphases, adsorption of gases by solids, type of adsorption, BET theorem, determination of surface area of solids, adsorption from solution.	**8**
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.	**8**
	Total	**42**

11. Suggested Books:

S.No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Barrow G.M., "Physical Chemistry", 4th Ed., McGraw Hill.	**1979**
2.	Rastogi R.P. and Sharma R.R., "Chemical Thermodynamics", Vikas Publishing House.	**1978**
3.	Moore W.J., "Physical Chemistry", 5th Ed., Orient Longman.	**1982**
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.	Mc Quarie, D. A., "Statistical Mechanics" Viva Books Pvt. Ltd	**2003**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code : **CYN-522** Course Title: **Kinetics and Photochemistry**
2. Contact Hours : **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) Theory **03** Practical **00**
4. Relative Weight: CWS **25** PRS **0** **MTE** 25 ETE **50**
5. Credits: **03** 6. Semester: **Spring** 7. Subject Are: **PCC**
8. Pre-requisite: **Nil**
9. Objective of Course: To impart basic knowledge to students of the kinetics and mechanism of thermal, photochemical and radiation chemical reactions.
10. Details of Course:

S.No.	Contents	Contact hours
1.	**Reaction Dynamics**: Arrhenius equation, the concept of activation energy, theoretical calculation of energy of activation using potential energy surface diagram, simple collision theory, 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 acid, base and enzyme catalysis, Hinshelwood mechanism of catalysis.	**16**
3.	**Photochemistry**: Quantum yield, actinometry-physical and chemical actinometers, experimental techniques for continuous photolysis. Electronic transition in organic molecules, photochemistry of carbonyl compounds – Norrish Type I and Norrish Type II cleavages, photoreduction, H-atom abstraction, photocycloaddition to ketones to ethylenes, Paterno-Büchi reaction, photochemistry of α, β-unsaturated ketones, esters, acids, benzoquinones, nitrite, photofries rearrangement, Barton reaction. Primary photophysical processes of atoms and diatomic molecules, spectroscopic notations, Franck-Condon principle and its applications, rates of absorption and emission, lifetimes of electronically excited states and its fate, quenching of excited states species, radiationless transition and predissociation, energy transfer processes, Wigner's spin rule, Woodward Hoffman's rule, mechanistic analysis of photochemical reactions by spectroscopic techniques, sources of high energy radiation, chemical dosimetry, comparison between photo- and radiation chemistry.	**16**
	Total	**42**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	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 International Pvt. Ltd., New Delhi.	**2004**
4	Turro N.J., "Modern Molecular Photochemistry", Benjamin Cumming Publications Co.	**1991**
5	Lakowicz J.R., "Principles of Fluorescence Spectroscopy", Plenum Press, New York.	**2003**
6	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 code: **CYN-531** Course Title: **Analytical Methods**
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** **ETE: 0**
5. Credits: **3** 6. Semester: **Autumn** 7. Subject Area: **PCC**
8. Pre-requisite: Nil
9. Objective: To impart the fundamental knowledge of different analytical methods

10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Atomic spectrometry**: Principle of atomic absorption and atomic emission spectrometry, instrumentation, atomic fluorescence spectrometry.	**7**
2.	**Separation methods**: Solvent extraction: Partition law and its limitations, distribution ratio, separation factor, factor influencing extraction, multiple extractions. Chromatography: theory of column chromatography, retention time, retention value, capacity factor, concept of plate and rate theory, resolution, column performance, paper and thin layer chromatography, ion exchangers.	**14**
3.	**Electroanalytical methods**: Polarography – principle, instrumentation, limitations, applications to qualitative and quantitative analysis, ameperometric and bioamperometric titrations	**7**
4.	**Nuclear methods**: Concept of radiotracers and radio labelling, radioisotope production and their properties, radioactivity and radiation measurement, activation analysis, isotope dilution method.	**14**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/Book/ Publisher etc.	Year of Publication/ Reprint
1.	Sood D.D., Reddy A.V.R. and Ramamoorthy N., " Fundamentals of Radiochemistry", Indian Association of Nuclear Chemists and Allied Scientists, BARC, Mumbai	**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.	Skoog D.A., West D.M., Holler F.J. and Crouch S.R., " Fundamentals of Analytical Chemistry" 8th Ed., Thomson Brooks/Cole.	**2004**
4.	Fifield F.W., and Kealey D., "Principles and Practice of Analytical Chemistry", 5th Ed., Blackwell Science.	**2000**
5.	Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill.	**2004**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-532** Course Title: **Advanced Organic Chemistry**
2. Contact Hour**:** **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory 03** **Practical 0**
4. Relative Weight: **CWS: 25** **PRS -** **MTE: 25** **ETE: 50**
5. Credits: **03** 6. Semester: **Spring** 7. Subject Area: **PCC**
8. Pre-requisite: **Nil**
9. Objective of Course: To impart advanced knowledge on reaction mechanism and pericyclic reactions.
10. Details of Course:

S.No	Contents	Contact Hours
1.	**Conformation and Chemical Reactivity**: Internal forces and strains, Conformational analysis of acyclic molecules (alkanes, halogeno alkanes and other substituted derivatives), conformational energy, diagrams, dynamic stereochemistry, reactivity of conformationally rigid and mobile diastereomers, quantitative correlation between conformation and reactivity, conformational analysis of cyclic system - mono, di and polysubstituted cyclohexanes , regiospecific, regioselective reactions, base-induced and pyrolytic eliminations, solvolysis, esterification, hydrolysis , oxidation, reduction, neighbouring participation reactions of acyclic and cyclic molecules. Brief idea on fused ring system- decalin , perhydroanthracene, perhydrophenanthrene and cyclopentanoperhydrophenanthrene	**14**
2.	**Organic reaction Mechanism**: Types of Mechanism, types of Reactions, importance of product analysis, reactive intermediates and their detection, information from reaction kinetics , reaction energetics, energy profile diagrams, activation parameters, isotope effects (primary and secondary kinetic hydrogen isotope effects), LFER-Hammett, Taft equations, solvent effects, kinetic and thermodynamic controls, Hammond postulates, guide lines for proposing reaction mechanism.	**14**
3.	**Pericyclic Reactions**: Orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allylic system, FMO approach, Woodward-Hoffman correlation diagram method, pericyclic reactions under thermal and photochemical conditions; electrocyclic reractions-conrotatory and disrotatory motions, [4n], [4n+2]allyl systems, cyclo addition-[4n], [4n+2] systems with emphasis on [2+2] and [4+2] cyclo additions,stereochemical and substituent effects, sigmatropic rearrangements-shifts of H and carbon moieties, detailed treatment of Claisen, Cope, Sommelet-Hauser rearrangements.	**14**
	Total	**42**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	Year of Publication/Reprint
1.	Eliel E.L., Samuel H.W. and Michael P.D., “Basic Organic Stereochemistry”, John Wiley & Sons.	**2001**
2.	Nasipuri D., “Stereochemistry of Organic Compounds”, Wiley Eastern Ltd., New Delhi.	**2005**
3.	Woodward R.B. and Hoffman R., The Conservation of Orbital Symmetry, Academic Press.	**2004**
4.	March J., Advanced Organic Chemistry, Reactions, Mechanism and Structure, John Wiley & Sons.	**2004**
5.	Bruckner R., “Advanced Organic Chemistry: Reaction Mechanism”, Academic Press.	**2002**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject : **CYN-541** Course Title: **Organic Chemistry**
2. Contact Hours : **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) Theory **03** Practical **0**
4. Relative Weight: CWS: **25** PRS - MTE: **25** ETE: **50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PCC**
8. Pre-requisite: **Nil**
9. Objective of Course: To introduce students with the concepts of spectroscopy, Stereochemistry, reactive intermediates and related concepts.
10. Details of Course:

S. No.	Contents	Contact hours
1	**Spectroscopy:** General introduction to UV, IR and NMR spectroscopy their application to identification of simple organic compounds. Shifts of bands with solvents, isolated and conjugated double bonds, Woodward – Fieser rules, polyenes, carbonyl compounds, aromatic systems. Stereochemical non-equivalence – diastereotopic and enantiotopic protons, use of deuterium oxide to identify exchangeable hydrogen atoms..	**14**
2	**Disconnection Approach:** Synthons and synthetic equivalents, definitions, guidelines, functional group interconversions, use of acetylenes and aliphatic nitrocompounds in organic synthesis; two-group C-C disconnections – Diels-Alder reaction, 1,3- & 1,5-difunctional compounds (Michael addition & Robinson annulation); order of events in organic synthesis, chemoselectivity, reversal of polarity (umpolung), cyclisation reactions, and amine synthesis.	**8**
3	**Organometallic compounds:** **Transition metals-mediated reactions:** Organocopper intermediates; reactions involving organopalladium intermediates – palladium-catalyzed nucleophilic substitution and alkylation, Heck reaction, palladium-catalyzed cross coupling, and carbonylation reactions; reactions involving organonickel compounds; reactions involving rhodium and cobalt; organometallic compounds with π-bonding. Carbon-carbon bond-forming reactions of compounds of boron, and tin: Synthesis and C-C bond-forming reactions of organoboron, and organotin compounds.	**8**
4	**Organo silicon- and sulphur chemistry:** **Silicon:** Silicon and carbon compared, silicon Baeyer-Villiger rearrangement, nucleophilic substitution at silicon, silyl ethers and alkyl silanes as protecting groups, aryl and vinyl silanes, migration of silicon from carbon to oxygen. **Sulphur:** Sulphur stabilized anions, thioacetals, allyl sulphides, sulphonium salts, sulphonium ylids, sulphur stabilized cations, chiral sulphoxides in synthesis.	**8**
5	**Introduction to petrochemicals:** First generation of petrochemicals, second generation of petrochemicals, third generation of petrochemicals, catalysis in petrochemical processes, future of petrochemicals.	**4**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Morrison R.T. and Boyd R.N., "Organic Chemistry", 6th Ed., Prentice Hall of India.	**2001**
2.	Solomons T.W.G. and Fryhle C.B., "Organic Chemistry", 8th Ed., Wiley Inc.	**2004**

3.	Silverstein R.M. and Webster F.X., "Spectroscopic Identification of Organic Compounds", 6th Ed., Wiley Inc.	**2002**
4.	Pavia D.L., Lampman G.M. and Kriz G.S., "Introduction to Spectroscopy", 3rd Ed., Harcourt Inc.	**2001**
5.	Maiti S., "Introduction to petrochemicals", 2nd Ed., Oxford & IBH.	**2002**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code : **CYN-542** Course Title : **Laboratory-II**

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

3. Examination Duration (Hrs.): **Theory: 00** **Practical: 12**

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

5. Credits : **6** 6. Semester : **Spring** 7. Subject Area: P**CC**

8. Pre-requisite: Nil

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

10. Details of Course:

Contents	Contact Hours
List of Experiments **Organic Chemistry:** 1. Qualitative analysis: Identification of binary mixtures of organic compounds. 2. Identification and characterization of organic compounds through m.p., derivatization, IR etc. 3. Extraction, isolation and purification of natural products: Application of soxhlet, column chrom. and TLC: (i) Pigments from spinach leaves, (ii) Piperine from black pepper, (iii) Caffeine from tea leaves. 4. Multistep synthesis, e.g.: (i) Benzophenone-benzophenone oxime – benzanilide, (ii) Benzoin, benzyl, benzilic acid, (iii) Diphenic acid, (iv) anthranilic acid.	**4 × 14**
Inorganic Chemistry: 5. Synthesis of potassium tris(oxalate)aluminate, potassium tris(oxalate)chromate and potassium tris(oxalate) 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. 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 and UV-visible spectroscopy. 7. Comparison of the 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. 8. 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), 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. 9. (i) Study of the complex formation between Fe(III) and thiocyanate/salicylic acid/ sulphosalcylic acid or between Ni(II) and o-phenonthroline, and (ii) find the formula. (iii) Determination of formation constant of the complex spectrophotometrically (Job's method and molar ratio method).	**4 × 14**
Physical Chemistry: 10. Analysis of a mixture of a metal cation by electroanalytical methods. 11. Determination of cations in soil/fertilizer by flame photometry. 12. Determination of cations in lubricating oils/alloys using AAS. 13. To calculate the surface energy of given organic liquid from surface tension versus temperature relationship. 14. To study the fluorescence quenching.	**4 × 14**

15. To determine the variation of miscibility of phenol in water with temperature and to find the critical solution temperature. 16. To determine ΔG, ΔH, and ΔS for the reaction, Zn (Hg)+2;AgCl(S)= ZnCl2(aq)+2Ag(s) from e.m.f measurements. 17. To determine the ionization constant of bromophenol blue indicator by spectroscopy.	
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	Shriner R.L., Hermann C.K.F., Morrill T.C., Curtin D.Y. and Fuson R.C., "The Systematic Identification of Organic Compounds", 8th Ed., John Wiley & Sons.	**2004**
6	Garland C.W., Nifler J.W. and Schoemaber D.P., "Experiments in Physical Chemistry", 7th Ed., McGraw-Hill International.	**2002**

- Some experiments require two-three turns.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-551** Course Title: **Coordination Chemistry**

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 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.	**Molecular Magnetism and 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 ligands, ferromagnetic, anti-ferromagnetic, ferromagnetic behaviour of transition metal compounds, molecule based magnetic materials.	**11**
	Total	**42**

11. Suggested Books:

S. No.	Name of Books / Authors	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.	Que J.L. and Tolman, W.B., "Comprehensive Coordination Chemistry", McCleverty, J.A., Meyer, T.J., Eds., Pergamon Press.	**1988**
4.	Purcell K.F. and Kotz J.C., "Inorganic Chemistry", Saunders, London.	**1977**
5.	Figgis, B.N., and Hitchman, M.A "Ligand Field Theory and Its Applications", Wiley Eastern Ltd.	**1999**
6.	Drago R.S., "Physical Methods in Inorganic Chemistry", W.B. Saunders Publishing Company, Philadelphia.	**1977**
7.	Huheey J.E., Keiter E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education, Inc	**2003**
8.	Atkins P., Overton T., Rourke J., Mark W. and Armstrong, F., "Shriver and Atkins' Inorganic Chemistry", 4th Ed, Oxford university press.	**2009**
9.	Lee J.D., " Concise Inorganic Chemistry", 5th Ed, Blackwell Science Ltd.	**1999**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-552** Course Title: **Electroanalytical Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory 03** **Practical: 0**
4. Relative Weight: **CWS: 25** **PRS: 0** **MTE: 25** **ETE: 50** **PRE: 0**
5. Credits: **03** 6. Semester: **Spring** 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.	**Basics of Polarography:** Polarography and advantages of using dropping mercury electrode. 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. Determination of number of electrons. 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 etc 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- C60, single wall and multi wall carbon nanotubes. Preparation and characterization of modified surfaces, Applications of sensors in doping.	**7**
4.	Polarographic and cyclic voltametric studies of coordination 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.	Authors/ Title/ Publisher	Year of Publication/Reprint
1.	Meites L., Polarographic Techniques, Interscience publishers, N.Y. Third Edition.	**1990**
2.	Lund and Baizer, Organic electrochemistry, Marcel Dekker, N.Y.	**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 Code : **CYN-561** Course Title: **Laboratory-I**

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

3. Examination Duration (Hrs.): **Theory: 00** **Practical: 12**

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

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

8. Pre-requisite: Nil

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

10. Details of Course:

Contents	Contact Hours
List of Experiments **Organic Chemistry:** 1. Experiment involving crystallization/ distillation/purification, e.g: (i) Phthalic acid from hot water (ii) Naphthalene form ethanol. 2. Simple synthesis of organic compounds, e.g.: (i) p-nitroacetanilide, (ii) p-nitroaniline, (iii) p-amino azobenzene, (iv) adipic acid from cyclohexene (v) cinnamic acid from benzaldehyde. 3. Estimations of organic functional groups, e.g.: (i) glucose (ii) phenol (iii) glycine etc. 4. Separation techniques: (TLC, column chrom., UV-Vis), e.g, (i) Determination of R_f values and purity of organic compounds using TLC. 5. Separate a binary mixture of organic compounds using column chromatography.	**4 × 14**
Inorganic Chemistry: 1. Semi-micro qualitative analysis involving 8 radicals including interfering radicals. 2. Estimation 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 Ni and Zn; Cu and Zn. 6. Synthesis of simple coordination compounds: (i) Chrome alum, (ii) tetraaminecopper(II) sulphate, (iii) $Fe(acac)_3$ (iv) $Mn(acac)_3$.	**4 × 14**
Physical Chemistry: 1. Viscometry: Measurement of viscosity of solutions of a polymer, and calculation of average molecular weight of a polymer. 2. Determination of standard reduction potential of Cu/Cu^{2+} and Zn/Zn^{2+} electrodes. 3. Determination of pk_1 and pk_2 of dibasic acids. 4. Kinetics of saponification of an ester. 5. Determination of specific and molar rotation of sucrose solution using polarimeter. 6. To study the kinetics of H^+-catalysed hydrolysis of sucrose using polarimeter. 7. Verification of Freundlich adsorption isotherm and Langmuir adsorption isotherm. 8. Study of oscillatory reactions. 9. Determination of the equilibrium constant for $Kl+l_2 = Kl_3$ reaction using partition method. 10. Determination of the dimerization constant of acetic acid/benzoic acid. 11. Study of variation of angle of rotation with concentration of sucrose/tartaric acid using polarimetry. 12. To determine the velocity constant for the saponification of ethyl acetate, using the conductance method at 30^0C.	**4 × 14**

13. Determine the fluorescence quantum yield of the given substance.	
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.	Shriner R.L., Hermann C.K.F., Morrill T.C., Curtin D.Y. and Fuson R.C., "The Systematic Identification of Organic Compounds", 8th Ed., John Wiley & Sons.	**2004**
6.	Garland C.W., Nifler J.W. and Schoemaber D.P., "Experiments in Physical Chemistry", 7th Ed., McGraw-Hill International.	**2002**

- Some experiments require two-three turns.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject : **CYN-562** Course Title: **Enantiomeric Separation**
2. Contact Hours : **L: 2** **T: 0** **P: 2/2**
3. Examination Duration (Hrs) Theory **02** Practical **0**
4. Relative Weight**:** **CWS: 20** **PRS: 20** **MTE: 20** **ETE: 40** **PRE: 0**
5. Credits: **03** 6. Semester: **Spring** 7. Subject Area: **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**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	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**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-572** Course Title: **Heterocyclic Chemistry**

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

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

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

5. Credits: **03** 6. Semester: **Spring** 7. Subject Area: **PEC**

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

9. Objective of Course: To give the students 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 & 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 in this kind of rings, reactants employed and orientation of the substituent on the ring.	10
3	**Benzoderivatives 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 Oxazoles, thiazoles, oxadiazoles, thiadiazoles, benzothiazoles, benzothiadiazoles, triazole, benzotriazole, pyrimidines, pyrazines, quinoxalines, triazines, etc.	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, organic semiconductors for thin-film transistors.	6
	Total	42

11. Suggested Books:

S.No.	Authors/ Title/ Publisher	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, volume 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, Volume II: Five-membered heterocycles, R. R. Gupta, M. Kumar and V. Gupta, 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
7	Acheson R. M., "An introduction to the chemistry of heterocyclic compounds,", 3rd Ed., John Wiley and Sons, New York.	1976

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-582** Course Title: **Chemical Applications of Nanoscale Materials**

2. Contact Hours: **L: 3** **T: 1** **P: 0**

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

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

5. Credits: **03** 6. Semester: **Spring** 7: Subject Area: **PEC**

8. Pre-requisite: **Nil**

9. Objective of the Course: To introduce various aspects of chemical applications of nanoparticles.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	Overview of nanomaterials and nanoscale metal Oxides.	**2**
2.	**Reactivity and Characteristics of Nanoparticles:** Increased reactivity of nanoscale materials, reasons for high reactivity, effect of size and shape of nanocrystals on reactivity, comparison of nanocrystalline versus macro-crystalline materials in terms of reactivity.	**5**
3.	**Metal Oxide Nanoparticles: A**erogel method to produce materials with very high surface area, textural studies, determination of size, defects in nanocrystalline metal oxides, comparison of nanoscale metal oxides with other porous materials such as zeolites, clays etc. Typical reactions used for testing reactivity; SO_2 and CO_2 adsorption, H_2S adsorption, CCl_4 adsorption, adsorption of stimulant molecules of chemical warfare agents.	**9**
4.	**Chemical Modification of Nano Metal Oxides:** Prevention of agglomeration, impregnation / incorporation of suitable chemical agents on the surface of nanoparticles, increasing dispersibility in solution.	**5**
5.	**Applications of Nano Metal Oxides and Modified Nano Metal Oxides as Adsorbents:** Adsorbents based on nanostructured materials, destructive adsorption, decontamination of toxic chemicals, detoxification of surrogates of chemical warfare agents, air purification, desulfurization, destruction of chlorinated compounds. Mixed metal oxides, Lewis acid incorporated nanocrystalline metal oxides, model reactivity studies using modified nanocrystalline metal oxides.	**13**
6.	**Biocidal Applications:** Killing bacteria, spores and other harmful germs using halogenated nanoparticles, mechanism of biocidal action, and advantages of using biocides based on nanoparticles.	**4**
7.	**Toxicology:** Concerns in using nanoparticles, inhalation toxicity, oral toxicity, governmental regulations, case studies on toxicology, precautions.	**4**
	Total	**42**

11. Suggested books:

S. No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1	Klabunde K.J. (Ed.), "Nanoscale Materials in Chemistry", Wiley-Interscience, NY.	**2001**
2	Schmid G. (Ed.), "Nanoparticles: From Theory to Application", Wiley-VCH, Weinheim.	**2004**
3	Rodriguez J.A. and Fernandez-Garcia M., (Ed.), "Synthesis, Properties and Applications of Oxide Nanomaterials", John Wiley, New York.	**2006**
4	Rao C.N.R., Müller A. and Cheetham A.K., "The Chemistry of Nanomaterials: Synthesis, Properties and Applications", (Volumes 1 and 2), Wiley-VCH Verlag, Weinheim.	**2004**

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: 12**
3. Examination Duration (Hrs.): **Theory 0** **Practical 12**
4. Relative Weight: **CWS 0** **PRS 50** **MTE 0** **ETE -** **PRE 50**
5. Credits: **06** 6. Semester : **Autumn** 7. Subject **Area**: P**CC**
8. Pre-requisite: **Nil**
9. Objective: To impart practical knowledge and skills in handling instruments in physical, inorganic and organic laboratories.
10. Details of Course:

Content	Contact Hours
List of Experiments **1. Electrochemical**: (a) Determination of metal ions by polarography. (b) Voltammetry of organic compounds using glassy carbon electrode and elucidation of nature of redox process. **2. Gas Chromatography**: Catalytic applications of metal complexes in oxidation reactions. **3. Flame Photometry**: To determine the concentration of Na (in ppm) in the given unknown solution with the help of flame photometer using (i) standard addition method and (ii) internal standard method. **4. IR/NMR/Mass**: Synthesis of organic compounds, their separation using column or other suitable chromatography and characterization. **5. Radiochemistry**: (a) Measurement of radio activity by GM counter and NaI detector. (b) Synthesis of ZnO nano particles and photocatalytic studies. **6. Spectrophotometry:** (a) Simultaneous spectrophotometric determination of Cr and Mn in a given sample. (b) To analyse aspirin in a commercial tablet using spectrophotometric and titrimetric methods. **7. Magnetic Measurements**: (a) Synthesis of iron/chromium complexes and their characterization by IR , UV-Vis spectrometry, magnetic measurements and photochemical studies.	**12 × 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	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 Text Book of Practical Organic Chemistry", 5th Ed., Longman.	**1996**
4	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: **CYN-611** Course Title: **Molecular Spectroscopy**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory 03** **Practical 00**
4. Relative Weight: **CWS 25** **PRS 0** **MTE 25** **ETE 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Elementary knowledge of molecular spectroscopy**
9. Objective of Course: To provide basic knowledge of various spectroscopic techniques required for the identification and elucidation of the structure of molecules.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Introduction to Spectroscopy:** Different aspects of molecular spectroscopy, the Born-Oppenheimer approximation, transition probability, oscillator strength, the integrated absorption coefficient.	**2**
2.	**Microwave Spectroscopy**: Classification of rotors, intensity of rotational lines, population of energy levels, non-rigid rotation, anharmonocity and centrifugal distortion, effect of isotopic substitution. Rotation spectra of linear, spherical top and asymmetric top polyatomic molecules, microwave technique.	**4**
3.	**Infrared Spectroscopy:** Vibrating rotor, vibration of polyatomic molecules, harmonic and anharmonic oscillators, types of vibration bands – overtones, combination bands, Fermi resonance phenomenon, the finger print region, FTIR spectroscopy and applications.	**4**
4.	**Raman Spectroscopy*:*** Rayleigh and Raman scattering, polarisabilities, rotational and vibrational Raman spectra, selection rules, polarization of the light and Raman effect, Laser Raman spectroscopy.	**4**
5.	**UV Visible Spectroscopy**: Electronic spectra, Franck-Condon Principle, predissociation spectra, Fortrat diagram. Electronic spectra of organic compounds, types of transitions, solvent effects, empirical rules of λ_{max}, conjugated polyene and enone systems, transition in inorganic complexes, charger transfer spectra in organic and inorganic systems.	**4**
6.	**Magnetic Resonance Spectroscopy**: Nuclear moments, nuclear spin states in a magnetic field and the resonance phenomenon, relaxation processes, Bloch equations outline of NMR detection methods; chemical shifts and spin-spin coupling, spectra of a two-spin system (A_2, AB and AX cases); interpretation of simple first order spectra of organic molecules. NMR lineshapes and molecular dynamics. FT-NMR spectroscopy, measurement of relaxation times, introduction to ^{13}C NMR spectroscopy.	**7**
7.	**Electron Spin Resonance:** detection of ESR spectra, spectra of simple organic radicals, g-values and hyperfine structure, the McConnell relation; spectra of inorganic complexes, zero field splitting and Krammers degeneracy. General introduction to double resonance experiments, Overhauser effect, DNDOR and ELDOR, 2-dimensional NMR, Zeugmatography and biological applications.	**6**
8.	**NQR and Mössbauer Spectra**: Nuclear quadrupole moment and EFG tensors, quadrupole coupling constants and asymmetry parameters, pure NQR and Zeeman spectra of spin 1/2 and spin 3/2 systems; the Towners-Dailey theory and interpretation of NQCC in terms of bond characteristics. The Mössbauer effect, isomer shifts and NQCC's ^{57}Fe spectra of complexes, other Mössbauer nuclei, applications.	**6**
9.	**Photoelectron Spectroscopy:** The photoionisation processes, Auger and autoionisation processes, deexcitation by fluorescence, cross-sections; outline of the XPS, UPS and Auger techniques and their applications: correlation with band structure of solids, application to organic molecules and surface structure studies.	**5**
	Total	**42**

11. Suggested books:

S. No.	Authors/ Title/ Publisher	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.	Flygare W.H., "Molecular Structure and Dynamics", Prentice Hall.	**1978**
3.	Slichter C.P., "Principles of Magnetic Resonance", Springer Verlag.	**1981**
4.	Graybeal J.D., "Molecular Spectroscopy", McGraw-Hill.	**1988**
5.	Atkins P. and Paula J.de, "Physical Chemistry", 7th Ed., Oxford Univ. Press.	**2003**
6.	Drago R.S., "Physical Methods in Inorganic Chemistry", Reinhold Publishing Corp., East West Press Pvt. Ltd.	**1986**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CY-621A** Course Title: **Advanced Analytical Chemistry I**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 03 Practical 00**
4. Relative Weight: **CWS 25 PRS - MTE 25 ETE 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Knowledge of analytical chemistry**
9. Objective of Course: To impart knowledge of advanced topics in analytical techniques
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Electroanalytical methods:** Principle, instrumentation and applications of pulse, rapid scan, square wave and AC polarography cyclic voltammetry, coulometry at controlled potential, chronopotentiometry and anodic stripping voltammetry.	**10**
2.	**Ion sensors:** semipermeable membranes, selectivity, different types of solid and liquid membrane sensors.	**5**
3.	**Spectral methods:** Principle, instrumentation and applications of atomic absortion, atomic emission and atomic fluorescence, beam modulation in AAS, spectral and chemical interferences in atomic spectroscopy, Arc/ spark, laser and plasma emission techniques, qualitative and quantitative analysis.	**10**
4.	**X-ray methods:** X-ray spectra, X-ray absorption, emission, fluorescence and diffraction methods, monochromatization, detection of x-rays, application of X-ray spectroscopy for analyses and characterization of materials, Particle Induced X-ray Emission, optical and electron microscopy.	**9**
5.	**Mass spectrometry:** Introduction, different types of ion sources, mass analysers and detectors, resolution and resolving power, interpretation of mass spectra, hyphenated systems – LC-MS, GC-MS, ICP-MS, MS-MS.	**8**
	Total	**42**

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.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., Pearson Education.	**2004**
2.	Skoog D.A., West D.M., Holler F.J. and Crouch S.R., "Fundamentals of Analytical Chemistry", 8th Ed., Thomson Brooks/Cole.	**2004**
3.	Fifield F.W. and Kealey D., "Principles and Practice of Analytical Chemistry", 5th Ed., Blackwell Science.	**2000**
4.	Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill Book Company, Inc.	**2004**
5.	Rochow T.G. and Tuckor P.A. "Introduction to microscopy by means of light, electron, X-rays or Acoustics", Springer, 2nd Ed.	**2005**
6.	Jenkins R., "X-ray fluorescence spectrometry (Chemical Analysis; A series of Monographs on Analytical Chemistry and its application", Wiley-Interscience, 2nd Ed.)	**1999**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-621I** Course Title: **Inorganic Biochemistry and Reaction Mechanism**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs): **Theory 03** **Practical 00**
4. Relative Weight: **CWS 25** **PRS 0** **MTE 25** **ETE 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
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. 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~~hae~~moglobin, myoglobin; non-porphyrin oxygen carriers~~hem~~erythrin, 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.	**5** **12**
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.	**8**
	Total	**42**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	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	**1991**

	Revised Ed., VCH, New York.	
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., Valentine J.S., "Bioinorganic Chemistry", University Science Books, U.S.A.	**1994**
6.	Lippard S.J., Berg J., "Principles of Bioinorganic Chemistry", University Science Books, U.S.A.	**1994**
7.	Geoffrey G.L., Wrighton M.S., "Organometallic Photochemistry", Academic Press.	**1979**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-621O** Course Title: **Advanced Organic Chemistry- I**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 03 Practical 0**
4. Relative Weight: **CWS: 25 PRS: 0 MTE : 25 ETE : 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Knowledge of organic chemistry**
9. Objective of Course: To bring student's knowledge the concepts of pharmaceuticals and biosynthesis of natural products.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Pharmaceuticals**: Introduction to the clinically used drugs such as sulphonamides, antimalarials, arsenical drus, antibiotics, the penicillins, cephalosporin C, streptomycin, chloramphenicol, macrolide group of antibiotics, polypeptide antibiotics. General pharmacology, qualitative aspects of drug action, receptors, quantitative aspects of drug-receptor interactions, therapeutic index, various modes of administration of drugs, gram positive and negative micro-organisms, NSAID's and their mode of action. Representative antibacterial drugs, anticancer, anti HIV drugs, their structure, mode of action.	**13**
2.	**Enzymes, coenzymes, fermentation**: Enzymes- classification, mode of action, key features of active site, Michaelis- Menten model for kinetic properties of enzymes, enzymic inhibition-competitive and non-competitive. Enzymic oxidation of simple biomolecules. Coenzymes- catalytic role of TPP, COASH, coenzyme-I, coenzyme-II, AMP,ADP,ATP,FMN, FAD and other high energy molecules, their biogenetics, coupled reactions.	**5**
3.	**Biogenetic pathways and Biosynthesis of Natural Products:** Acetate pathway- biosynthesis of fatty acids, coenzyme-A and its role, prostaglandins and physiological activities, poly ketides, biosynthesis of aromatic compounds, tetracyclines. Mevalonate pathway-biosynthesis of isoprenoids,mono and sesquiterpenes, bicyclic diterpenes, kaurene, gibberellic acid, squalene, biosynthesis of steroids, lanosterol, zymosterol, cholesterol, calciferol, stigmasterol and their biological activities. Phytoene-biosynthesis α, β, γ carotenes and other carotenoids, 11-cis-Retinal and its biological role. Shikimic acid pathway- Biosynthesis of aliphatic and aromatic amino acids, coumarins,lignans, flavones, isoflavones, flavanones,anthocyanidins **Biosynthesis of alkaloids:** alkaloids of the pyrrolidine and piperidine series ,nicotine, anabasine, tropine, atropine, cocaine ,sedamine , coniine, amphetamine, mescaline, ephedrine, dopamine, thebaine, codeine, morphine,serotonin, melatonoin and other physiologically active alkaloids	**13**
4.	**Nucleic acids**: Human Genome project , Structure and synthesis of nucleosides and nucleotides, DNA sequencing, DNA, replication of DNA, mutation, genetic code, role of nucleic acid in the biosynthesis of proteins, DNA finger printing , DNA modification and chemical carcinogenesis, P.C. reactions	**11**
	Total	**42**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	Year of Publication/Reprint
1.	Dewick P.M., "Medicinal Natural Products: A Biosynthetic Approach", John Wiley & Sons.	**2002**
2.	Mann J., "Chemical Aspects of Biosynthesis", Oxford Univ.Press.	**2002**

3.	Stryer L., Berg J.M. and Tymoczko J.L. "Biochemistry", W.H. Freeman & Co. NY.	**2002**
4.	Nelson D.L. and Cox M.M., "Lehninger Principles of Biochemistry" W.H. Freeman & Company. NY.	**2005**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-621P** Course Title: **Advanced Physical Chemistry - I**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 03 Practical 00**
4. Relative Weight: **CWS 25 PRS 0 MTE 25 ETE 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Knowledge of physical chemistry**
9. Objective of Course: To familiarize the students with advanced types of physical chemistry.
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 its applications, macro and micro emulsions, dispersion and aggregation of solids by surfactants.	**9**
2.	**Membranes**: Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.	**6**
3.	**Adsorption:** Model for multilayer adsorption, BET isotherm, adsorption by porous, non-porous and microporous solids, estimation of specific surface and pore size distribution, special problems encountered with very narrow pores, adsorption from liquid phase.	**9**
4.	**Colloids:** Electrical double layer and its structure, electro-kinetic potential, Verwey-Overbeek treatment of rapid and slow coagulation, properties and structure of gels, rheology, clay colloids.	**6**
5.	**Macromolecules:** Concepts of mass and number average molecular weights, methods of determining molecular weights (osmometry, viscometry, diffusion and light scattering method), sedimentation, frictional 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.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Rosen M.J., "Surface and Interfacial phenomena", John Wiley & Sons, N.Y.	**1978**
2.	Moody G.J. and Thomas J.D., "Selective Ion Sensitive Electrodes", Merrow Publishing Company Ltd., Watford, England.	**1971**
3.	Kruyt, H.R., "Colloid Chemistry", Vol I & II, Elsevier	**1952**
4.	Gregg, S.J. and Sing, K.S.W., "Adsorption, Surface Area and Porosity", 2nd Ed., Academic Press.	**1982**
5.	Adamson, A.W., "Physical Chemistry of Surfaces", 5th Ed., John Wiley & Sons, N.Y.	**1990**
6.	Billmeyer, F.W., "Text book of Polymer Sciences", 3rd Ed., Wiley, N.Y.	**1984**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-631A** Course Title: **Advanced Analytical Chemistry II**
2. Contact Hours: **L: 3 T; 0 P: 0**
3. Examination Duration (Hrs): **Theory 03 Practical 00**
4. Relative Weight: **CWS 25 PRS - MTE 25 ETE 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Knowledge of analytical Chemistry**
9. Objective of Course: To impart knowledge of advanced analytical techniques
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Radiometric methods of analysis:** Activation methods of analysis – neutron sources, thermal and fast neutron activation, prompt gamma, charged particle and photon activation, theoretical and experimental considerations, sources of error, advantages, limitations and applications. Isotope dilution and substoichiometric analysis - advantages, limitations, and applications, instrumentation and advantages, radioimmunoassay and radio reagent methods, Positron emission spectroscopy. **Analytical Methods using particle accelerator**: Rutherford Backscattering Spectrometry and its applications to material characterization, Nuclear Microprobe and applications, Introduction to Accelerator Mass Spectrometry – a modern dating method.	**13**
2.	**Liquid-liquid extraction:** Principle, significance of various terms, batch and counter current extraction, classification of extractants, extraction equilibria of metal chelate, ion association complexes, extraction by high molecular weight amines, synergism, stripping, backwashing, salting out agents, masking agents, emulsion formation, identification of extracting species.	**9**
3.	**Chromatographic techniques:** Plate concept, processes leading to non-ideal chromatography, van Deemter equation, plate height equation, Kovats index, high pressure liquid chromatography, bonded phase, instrumentation, detector characteristics, ion chromatography, revere phase chromatography, size exclusion chromatography, affinity chromatography.	**10**
4.	**Ion exchange:** Introduction, kinetic and thermodynamic considerations in ion-exchange, synthetic inorganic ion-exchangers – classification and applications, ion exchange in mixed aqueous organic media, chelating resins.	**5**
5.	**Automation in microanalysis:** Automation in analytical chemistry – automatic and automated devices instrumental parameters, principles and techniques of automatic analysers employed for microanalysis with emphasis on the basic sequences in operational modes in segmented and continuous flow, non-destructive autoanalysers in quality control. Elemental analysers, application in environmental and clinical laboratory	**5**
	Total	**42**

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.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., Pearson Education.	**2004**
2.	Skoog D.A., West D.M., Holler F.J. and Crouch S.R., "Fundamentals of Analytical	**2004**

	Chemistry", 8th Ed., Thomson Brooks/Cole.	
3.	Christian G.D., "Analytical Chemistry", 6th Ed., John Wiley & Sons Inc.	**2004**
4.	Fifield F.W. and Kealey D., "Principles and Practice of Analytical Chemistry", 5th Ed., Blackwell Science.	**2000**
5.	Ewing G.W., "Instrumental Methods of Chemical Analysis", 5th Ed., McGraw Hill Book Company, Inc.	**2004**
6.	Ehmann W.D. and Vance D.E., "Radiochemistry and Nuclear methods of Analysis", Wiley- InterScience, new Ed.	**2007**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-631I** Course Title: **Solid-State Chemistry and its Applications**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 3 Practical 00**
4. Relative Weight: **CWS 25 PRS 0 MTE 25 ETE 50**
5. Credits: **03** 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 characterization methods for metal complexes.
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Crystal Structure of Inorganic Compounds:** Crystalline solids, overview of close packing, packing efficiency, cubic, octahedral and tetrahedral interstitial sites, limiting radius ratios, method of determination of ionic radii. **Ionic Crystals Containing Two Different Elements:** Cesium chloride, rock-salt, zinc blende, wurtzite, fluorite, antifluorite, nickel-arsenide, CaC_2, CdI_2 and rutile structures. **Ionic Crystals Containing 3 Different Elements:** Ilmenite, spinels, inverse spinels, garnets perovskite and $KNiF_3$. **Non-ionic crystals:** Giant molecules, layer structure, crystals composed of discrete molecules.	**15**
2.	**Defect Structures:** Schottky and Frenkel defects, solid electrolytes, non-stoichiometric compounds, F-centers and other defects in non-stoichiometric compounds.	**3**
3.	**Methods to Synthesize Solid-state Materials:** Hydrothermal, sol-gel, co-precipitation (precursor), ceramic method. Different methods to grow single crystals.	**3**
4.	**Amorphous Inorganic Materials:** Glasses, refractories, materials obtained from organometallic chemical vapour deposition (OCVD). **New materials**: Conducting polymers, carbon nanotubes, carbon nanorods and fullerenes. **Electronic materials**: Insulating, semiconducting, superconducting materials, ferroelectrics, dielectrics.	**5**
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, etc), 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).	**10**
	Total	**42**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	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.	Cotton F.A., Wilkinson G., Murillo C.A. and Bochmann M., "Advanced Inorganic	**1999**

	Chemistry", 6th Ed., John Wiley & Sons, New York.	
3.	West A.R., "Solid State Chemistry and its Applications", John Wiley & Sons, New York.	**1989**
4.	Smart L. and Moore E., "Solid State Chemistry: An Introduction", Nelson Thornes Ltd.	**2001**
5.	Rao C.N.R. and Gopalakrishnan J. (Ed.), "New Directions in Solid State Chemistry", Cambridge University Press, Cambridge.	**1997**
6.	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-631O** Course Title: **Advanced Organic Chemistry II**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory 03** **Practical 00**
4. Relative Weight: **CWS: 25** **PRS 0** **MTE : 25** **ETE : 50**
5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Knowledge of spectroscopy**
9. Objective of Course: To familiarize students with the use of spectroscopy through structure determination and to design organic synthesis
10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Structure and Synthesis of Outstanding Organic Molecules:** Penicillins, newer penicillins, tetracycline, camphor, abietic acid, gibberellic acid, morphine, quinine, cortisone, prostaglandins, quercetin, vitamins.	**21**
2.	**Determination of structures of complex organic molecules by spectroscopic means:** Introduction, Coupling – vicinal and geminal coupling, long-range coupling, spin decoupling, spin systems - AX_2, A_2B_2 & A_2X_2 and AMX, ABX, & ABC types. Homotopic, enantiotopic and diastereotopic systems, chemical shift reagents, chiral resolving agents, NOE difference spectra, ^{19}F, ^{31}P NMR. 2D NMR – Introduction, NOESY, COSY, HETCOR, Carbon-13 NMR spectroscopy. Detailed study of mass spectroscopy.	**21**
	Total	**42**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Morrison R.T. and Boyd R.N., "Organic Chemistry", 6th Ed., Prentice Hall of India.	**2001**
2.	Solomons T.W.G. and Fryhle C.B., "Organic Chemistry", 8th Ed., Wiley Inc.	**2004**
3.	Finar I.L., "Organic Chemistry", Vols. 1 & 2, 6th Ed., ELBS Longman Ltd.	**1997**
4.	Singh J. and Yadav L.D.S., "Organic Synthesis", Pragati Prakashan.	**2006**
5.	Silverstein R.M. and Webster F.X., "Spectroscopic Identification of Organic Compounds", 6th Ed., Wiley Inc.	**2002**
6.	Pavia D.L., Lampman G.M. and Kriz G.S., Introduction to Spectroscopy, 3rd Ed., Harcourt Inc.	**2001**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-631P** Course Title: **Advanced Physical Chemistry - II**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 03 Practical 00**
4. Relative Weight: **CWS 25 PRS 0 MTE 25 ETE 50**
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, kinectics – proton transfer and electron transfer reactions, fast reactions – rapid flow, stopped – flow and relaxation techniques, molecular beam method, diffusion controlled reactions, oscillatory reactions, LFER and kinetic isotope effects, 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	**Quantum Chemistry:** Dirac Braket 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.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Laidler K.J., "Reaction Kinetics", Anand Sons, New Delhi.	**2005**
2.	Melander L. and Saunders W.H., "Reaction Rates of Isotopic Molecules".	**1980**
3.	Kondepudi D. and Prigogine I. , "Modern Thermodynamics: From Heat Engines to Dissipative Structures", John Wiley & Sons	**1998**
4.	Callen H. B., "Thermodynamics and an Introduction to Thermostatistics", John Wiley and Sons.	**1985**
5.	Bransden B.H., Joachain C.J., "Quantum Mechanics", Addison-Wesley.	**2000**
6.	Sakurai J. J., "Modern Quantum Mechanics", Pearson Education.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-641** Course Title: **Asymmetric Synthesis**

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

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

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

5. Credits: **03** 6. Semester **Autumn** 7. Subject Area: P**EC**

8. Pre-requisite: **Organic Chemistry**

9. Objective of Course: The course is designed to familiarize the student with the principles and applications of asymmetric synthesis.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Introduction**: Significance of chirality and stereoisomeric discrimination, asymmetry, determination of enantiomer composition, determining absolute configuration, general strategies for asymmetric synthesis, common definitions in asymmetric synthesis and stereochemistry.	4
2.	**α-Alkylation and Catalytic Alkylation of Carbonyl Compounds:** Chirality transfer (intra-annular, extra-annular and chelation-enforced intra-annular); preparation of quaternary carbon centers and α-amino acids; nucleophilic substitution of chiral acetal; chiral catalyst induced aldehyde alkylations: asymmetric nucleophilic addition; catalytic asymmetric additions of diethylzinc to ketones; asymmetric cyanohydrination and α-hydroxyphosphonylation.	5
3.	**Aldol and Related Reactions:** Substrate-controlled aldol reactions: oxazolidones, pyrrolidones, aminoalcohols and acylsultam systems as chiral auxiliaries; reagent-controlled aldol reactions: aldol condensations induced by chiral boron compounds, aldol reactions controlled by Corey's reagents, aldol condensations controlled by miscellaneous reagents; chiral catalyst-controlled aldol reactions: Mukaiyama's system, asymmetric aldol reactions catalyzed by chiral Lewis acids, catalytic asymmetric aldol reaction promoted by bimetallic catalysts (Shibasaki's system); double asymmetric aldol reactions; asymmetric allylation reactions; asymmetric allylation and alkylation of imines; Henry reaction.	6
4.	**Asymmetric Oxidations: Asymmetric Epoxidation of Allylic Alcohols:** Sharpless epoxidation; characteristics, mechanism and modifications and improvements of Sharpless epoxidation; selective opening of 2,3-epoxy alcohols: opening by external nucleophiles, intramolecular nucleophiles, metallic hydride reagents and organometallic compounds; Payne rearrangement, asymmetric desymmetrization of *meso*-epoxides; asymmetric dihydroxylation and aminohydroxylation of olefins; epoxidation of unfunctionalized olefins: catalytic enantioselective epoxidation of simple olefins by salen complexes and by porphyrin complexes; chiral ketone-catalysed asymmetric oxidation of unfunctionalised olefins; catalytic asymmetric epoxidation of aldehydes; asymmetric oxidation of enolates: substrate- and reagent-controlled reactions; asymmetric aziridination and regioselective ring opening of aziridines.	5
5.	**Asymmetric Diels-Alder and Other Cyclization Reactions***:* Chiral dienophiles: acrylate, α,β-unsaturated ketone, chiral α,β-unsaturated N-acyloxazolidinones, chiral sulfinyl-subtituted compounds; chiral dienes; double asymmetric cycloaddition; chiral Lewis-acid catalysts: Narasaka's catalyst, chiral lanthanide catalyst, bissulfonamides chiral acyloxy borane catalysts, Brønsted acid-assisted chiral Lewis-acid catalysts, bis(oxazoline) catalysts; hetero Diels-Alder reactons: oxo- and aza-Diels-Alder reactions; intramolecular and retro-Diels-Alder reactions; asymmetric dipolar cycloaddition and asymmetric cyclopropanation.	6
6.	**Asymmetric Catalytic Hydrogenation and Other Reduction Reactions**: Chiral phosphine Ligands for homogeneous asymmetric catalytic hydrogenation synthesis, asymmetric catalytic	5

	hydrogenation of C=C bonds; asymmetric reduction of carbonyl compounds: reductions using BINAL-H, transition metal-complexes and oxazaborolidine catalyst systems; asymmetric reduction of imines; asymmetric transfer of hydrogenation and asymmetric hydroformylation.	
7.	**Biocatalysis:** Introduction, hydrolases – lipases, esterases and proteases in organic synthesis	**3**
8.	**Asymmetric Organocatalysis**: Introduction; nucleophilic addition to electron-deficenet C=C double bonds: intermolecular Michael addition (C-, N-, O-, S-, and Se-nucleophiles), intramolecular Michael addition; nucleophilic addition to C=N double bonds: Strecker reaction (chiral diketopiperazines, guanidines, ureas and thioureas, N-oxides as catalysts), Mannich reaction (direct Mannich reaction – products with one and two stereogenic centers), β-lactam synthesis, aziridination and hydophosphonylation of imines; nucleophilic addition to C=O double bonds: hydrocyanation, aldol reactions, β-lactone synthesis via ketene addition, Morita-Baylis-Hillman reaction, allylation reaction, Darzens reaction; cycloaddition reactions: Diels-Alder, hetero-Diels-Alder reactions, dipolar cycloaddition reaction; large scale applications of ogeneral aspects and considerations, economy of catalyst, stability of catalyst and handling and recycling issues, conversion and catalytic loading.	**8**
	Total	**42**

11. Suggested books:

S. No.	**Authors/ Title/ Publisher**	**Year of Publication/ Reprint**
1.	Lin G.-Q., Li Y.-M. and Chan A.S.C., "Principles and Applications of Asymmetric Synthesis", Wiley.	**2001**
2.	Berkessel A. and Gröger H., "Asymmetric Organocatalysis" Wiley.	**2005**
3.	Ojima I.(Editor), "Catalytic Asymmetric Synthesis", 2nd Ed., Wiley.	**2004**
4.	Rizzacasa M.A. and Perkins M., "Stoichiometric Asymmetric Synthesis", Academic Press.	**2000**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

Subject: **CYN-651** Course Title: **Crystal and Molecular Structure**

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

3. Examination Duration (Hrs) **Theory 02 Practical 0**

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

5. Credits: **03** 6. Semester: **Autumn** 7. Subject Area: **PEC**

7. Pre-requisite: **Nil**

8. Objective of Course: To highlight relationship between symmetry, structure and properties and molecular structure determination.

10. Details of Course:

S.No.	Contents	Contact Hours
1.	**Crystallography**: Concept of crystallinity, elements of repetition and space symmetry, crystal systems and space groups.	**4**
2.	**X-ray crystallography**: X-ray diffraction from one, two- and three dimensional array of atoms; structure factor, systematic absences in x-ray diffraction pattern, Bragg equation, powdered method of x-ray diffraction, indexing of powdered pattern of cubic, tetragonal and hexagonal materials, applications of powdered x-ray diffraction pattern, reciprocal lattice, single crystal methods – rotating crystal, Weissenberg camera and precessional camera methods, single crystal x-ray diffractrometer, indexing of diffraction photographs.	**12**
3.	**Structure Analysis**: Treatment of diffraction data, phase problem, observed and difference Fourier synthesis, Patterson synthesis, statistical methods of phasing, refinement of structure.	**6**
4.	**Electron Diffraction**: Wave nature of electrons, scattering of electrons, experimental set-up, Mark and Wierl equation, scattering intensity curves, applications of electron diffraction.	**3**
5.	**Neutron Diffraction:** Neutron sources and detection of neutrons, scattering cross sections, applications to the studies of molecular structure.	**3**
	Total	**28**

11. Suggested books:

S.No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Ramakrishnan V. and Gopinathan M.S., "Group Theory in Chemistry", 2nd Ed., Vishal Publications.	**2000**
2.	Drago R.S., "Physical Methods in Inorganic Chemistry", East West Press Pvt. Ltd	**1986**
3.	Atkins P. and Paula J.de, "Physical Chemistry", 7th Ed., Oxford University Press.	**2002**
4.	Buerjer M.J., "Crystal Structure Analysis", John Wiley & Sons, New York.	**1987**
5.	Mass W., "Crystal Structure Determination", Springer-Verlag, Berlin, Heidelberg.	**2004**
6.	Cotton F.A., "Chemical Applications of Group Theory", John Wiley & Sons.	**1992**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject: **CYN-661** Course Title: **Organic Semiconductors: Synthesis and Applications**

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

3. Examination Duration (Hrs) **Theory 03** **Practical: 00**

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

5. Credits: **03** 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, polyphenylenevinylenes, polyphenyeleneethynylenes, polyfluorenes, polythiophenes, polyphenylenes, 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.	Authors/ Title/ Publisher	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 Solids", Cambridge University Press.	**2006**
4.	Schubert E.F., "Light-Emitting Diodes", Cambridge University Press, 2nd Ed.	**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**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject : **CYN-671** Course Title: **Proteins and Polypeptides**
2. Contact Hours : **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs) **Theory 03** **Practical 00**
4. Relative Weight: **CWS 25** **PRS 0** **MTE 25** **ETE 50**
5. Credits: **03** 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-ecllulose, CM-cellulose etc.) HPLC.	**8**
3.	**Fragmentation of Polypeptides:** Chemical Methods – clearvage 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 etc.	**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–** in the structural analysis of Peptides and Proteins.	**3**
6.	Introduction of X-ray crystallography and electron microscopy.	**3**
7.	Peptide mapping and prediction of peptide and protein structure.	**3**
8.	Peptide synthesis including solid-phase and automated synthesizers.	**3**
	Total	42

11. Suggested books:

S.No.	Authors/ Title/ Publisher	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-681** Course Title: **Supramolecular Chemistry**
2. Contact Hours: **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 03 Practical 0**
4. Relative Weight: **CWS 25 PRS 0 MTE 25 ETE 50**
5. Credits: **03** 6. Semester: A**utumn** 7. Subject Area: **PEC**
8. Pre-requisite: **Basic chemistry and spectroscopy**
9. Objective of Course: Supramolecular chemistry is a new emerging domain lying amidst chemistry, biochemistry, physics, and materials science. The course will be a journey from the chemistry of the entities generated by intermolecular noncovalent interactions into their application in electronic devices.
10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Fundamentals of Supramolecular Chemistry:** Definitions, brief overview and examples; types of noncovalent 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, enantioselective 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, etc.	**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:** Supramolecular catalysis; membrane transport; sensors; phase-transfer catalysis; supramolecular devices and switches; memories, logic gates and related systems; molecular scale machines (mechanical rotors, gears, brakes, etc.; conversion of light into fuels and light into electricity.	**12**
	Total	**42**

11. Suggested Books:

S.No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Steed J.W. and Aswood J.L., "Supramolecular Chemistry", Wiley.	**2000**
2.	Beer P.D., Gale P.A. and Smith D.K., "Supramolecular Chemistry", Oxford Chemistry Printers, ISBN-10: 0-19-850447-0.	**1999**
3.	Cragg P., "A Practical Guide to Supramolecular Chemistry", Wiley-VCH, ISBN: 0-470-86654-3.	**2005**

4.	Schneider H.J. and Yatsimirsky A, "Principles and Methods in Supramolecular Chemistry", Wiley-VCH, ISBN: 0-471-97253-3.	**2000**
5.	Dodziuk,H., "Introduction to Supramolecular Chemistry", Springer, ISBN 1402002149.	**2001**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject : **CYN-691** Course Title: **Frontiers in Inorganic Biochemistry**
2. Contact Hours : **L: 3 T: 0 P: 0**
3. Examination Duration (Hrs) **Theory 03 Practical: 00**
4. Relative Weight: **CWS 25 PRS 0 MTE 25 ETE 50**
5. Credits: **03** 6. Semester: **Spring** 7. Subject Area: P**EC**
8. Pre-requisite: **Nil**
9. Objective of Course: The course will deal with frontier areas in inorganic biochemistry. Metalloproteins from cellular and molecular biological point of view will be discussed along with structural biology of metalloproteins.
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: (i) Iron-Sulphur Proteins (ii) 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, acetylene coenzyme synthetase (ACS), DAP1 **Heme:** Catalytic mechanism of Nitric Oxide Synthease and Heme Oxygenase,	**5**
5.	**Metal ions and Disease:** 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 15N and 13C, 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.	Authors/ Title/ Publisher	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 OF DEPTT./ CENTRE: **DEPARTMENT OF CHEMISTRY**

1. Subject Code: **CYN-711** Course Title: **Laboratory I**

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

3. Examination Duration (Hrs.): **Theory: 0** **Practical: 6**

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

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

8. Pre-requisite**: Nil**

9. Objective: To develop experimental skills for different approaches of characterization.

10. Details of Course:

S. No.	Contents
	List of Experiments:
1.	Simultaneous polarographic determination of two metal ions.
2.	Polarogaphic estimation of colouring matters in food and dyes.
3.	Use of atomic absorption spectroscopy in the estimation of metal contents in samples.
4.	Experiment based on the use of radiotracers, and radioactivity measurements.
5.	Experiment on separation and estimation of organic compounds using gas chromatograph.
6.	Multi-step synthesis and characterization of pharmaceutical drug.
7.	Analysis of organic components in a mixture by HPLC.

11. Suggested Books:

S. No.	Authors/ Books/ Publisher	Year of Publication/ Reprint
1.	Willard H.H. Merritt L.L., Dean J.A. and Settle F.A., "Instrumental Methods of Analysis",7th Ed., Wadsworth Publishing Co.	**1988**
2.	West A.R., "Solid State Chemistry and its Applications", John Wiley & Sons.	**1988**
3.	Arnikar H.J., "Essentials of Nuclear Chemistry", Wiley-Eastern.	**1990**
4.	Skoog D.A., Holler F.J. and Crouch S.R., "Principles of Instrumental Analysis", 6th Ed., Thomson Brooks.	**2007**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-712** Course Title: **Laboratory - II**

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

3. Examination Duration (Hrs.): **Theory 0** **Practical 6**

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

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

8. Pre-requisite**: Nil**

9. Objective: To develop experimental skills in modern methods of characterization.

10. Details of Course:

S. No.	Contents
	List of Practicals
1.	Use of IR spectroscopy in determination of the purity of commercial samples.
2.	Thermal decomposition studies of inorganic compounds and polymers.
3.	Magnetic measurements by vibrating sample magnetometer (VSM).
4.	Powdered x-ray diffraction pattern of a cubic/tetragonal system and indexing of the pattern (a) Determination of unit cell parameter. (b) Determination of number of molecules in a unit cell. (c) Identification of materials in a solid mixture by powder x-ray diffraction pattern.
5.	Preparation, characterization and photodegradation by ZnO nanoparticles.
6.	Study of flow behavior of different kind of viscous materials using rheometer.
7.	Determination of Caffeine in beverages by HPLC/ LC-MS.
8.	Synthesis of organic compounds and NMR studies.

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/ Reprint
1.	Radd M. and Palmer R. "Structure Determination by X-ray Crystallography", 4th Ed., Springer.	**2003**
2.	Willard H.H., Merritt L.L., Dean J.J. and Settle F.A., "Instrumental Methods of Analysis", 7th Ed., Wadsworth Publishing Co.	**1988**
3.	Skoog D.A., Holler F.J. and Crouch S.R., "Principles of Instrumental Analysis", 6th Ed., Thomson Brooks.	**2007**
4.	Ewing G.W., "Instrumental Methods of Chemical Analysis**",** 5th Ed**.,** McGraw**-**Hill**.**	**2006**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-721** Course Title: **Analytical Methods**

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

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

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

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

8. Pre-requisite**: Nil**

9. Objective: To impart advanced knowledge of different methods of analysis as applied in industry and research.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Chromatographic Methods:** General principles of chromatography, retention, resolution and separation factor, place concept, van Deemter equation, chromatographic column and detector characteristics; applications in quantitative analysis-Kovat's index; High Performance Liquid Chromatography (HPLC)- instrumentation, separation columns, detectors, interfacing with Gas Chromatography (GC) and HPLC with mass spectrometry; Reverse phase chromatography; Ion chromatography- its comparison with ion exchange, applications; Inorganic ion exchangers- their classification and application in radioactive waste processing; Affinity chromatography and gel filtration chromatography- basic principles and applications.	**12**
2.	**Electroanalytical Methods and Sensors:** Voltametric, coulometric methods; Principle, instrumentation, analytical applications of polarography, pulse and differential pulse polarography, cyclic voltammetry and alternating current cyclic valtammetry, chronopotentiometry, anodic and cathodic stripping voltammetry, microelectrodes, modified electrodes and their analytical applications, electro-separations at controlled potential; Membranes, electroactive materials, membrane potential, selectivity coefficients and their determination, discussion of some important ion and molecule sensors, applications.	**12**
3.	**Nuclear Analytical Methods:** Basic principle of methods based on radioactivity measurements, choice of radiotracers, advantages and limitations; Activation methods-neutron activation methods, principle, classification, methodology, instrumentation, multi-elemental and nondestructive character, interferences, cyclic and derivative activation analysis, typical applications for trace element analysis of various matrices, isotope dilution analysis (IDA) using radiotracers and stable isotopes, (ID-MS)- basic principle and methodology, limitations, comparison with neutran activation analysis (NAA), substoichiometric IDA; Other radiometric methods using radio-reagents, radiometric titration, radio-chromatography, radioimmunoassay, their advantages and applications; Radio isotopes in diagnosis and therapy.	**12**
4.	**Automation in Analysis:** Requirements of automation, automatic and automated devices, continuous and discrete analyzers, feedback control loop, on-line analyzer, automated process control, non-destructive automatic analyzer, automation in clinical, environmental analysis and quality control, automated elemental analyzers, laboratory robots.	**6**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Books/ Publisher	Year of Publication/ Reprint
1.	Willard H.H., Merritt L.L., Dean J.A. and Settle F.A., "Instrumental Methods of Analysis", 7th Ed., Wardsworth Publishing Co.	**1988**
2.	Vandecasteele C. and Block C.B., "Modern Methods of Trace Element Determination", John Wiley & Sons	**1993**
3.	Ehmann W.D. and Vance D.E., "Radiochemistry and Nuclear Methods of Analysis", John Wiley & Sons	**1991**
4.	Skoog D.A., Holler F.J. and Nieman T.A., "Principles of Instrumental Analysis" 5th Ed., Harcourt Brace & Company	**2006**
5.	Meites, L., "Polarographic Techniques", Interscience Publisher,	**2001**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-722** Course Title: **Pharmaceutical Organic Synthesis**

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**: Spring** 7. Subject Area**: PEC**

8. Pre-requisite**: Nil**

9. Objective: To provide an advanced knowledge of organic synthesis required in pharmaceuticals.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Biosynthesis vs Laboratory Synthesis:** Involvement of nucleic acids, amino acids, carbo-hydrates and lipids as drug targets, differences between laboratory synthesis and biological synthesis, mechanisms in biological chemistr: reductive amination, Michael addition, rearrangements, Shikimate pathway, secondary metabolites and their applications in pharmaceutic industry.	**6**
2.	**Strategies in Organic synthesis of drugs:** Disconnection approach, applications in 1,1-, 1,2-, 1,3- and 1,5-difunctionalized compounds, recognition of high yielding steps and recognizable starting materials, biomimetic approach to retrosynthesis, application of the disconnection strategies to the synthesis of propoxycaine, dinocap, (+)disparlure, retronecene, longifoline.	**8**
3.	**Green Chemistry Approach:** Principal, atom economy and scope, introduction to alternative approaches, solvent free reactions-principal, scope, utility, organic synthesis in solid state, solid supported organic synthesis-synthesis of aziridines, pyridines, chromenes and flavones, aqueous phase reactions: Diels Alder, Heck reaction, epoxidation, microwave technology: equipment, activation benefit, limitations, microwave effects in synthesis, microwave assisted solid phase reactions, neat reactions, microwave assisted reactions under PTC conditions, ultrasound assisted reactions: principal, benefits and limitations, ultrasound assisted substitution, addition, oxidation and reduction reactions, organocatalysis: Aldol reaction, acyl transfer reactions, setter reaction, Bakers yeast, N-heterocyclic carbenes, ionic liquids: introduction and application in organic synthesis.	**14**
4.	**Total synthesis**: Corey's synthesis of prostaglandins and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of Taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.	**6**
5.	**Scaffolds in Pharmaceutical Synthesis:** Diversity in pharmaceutical scaffolds, diversity oriented synthesis, synthesis, reactivity, aromatic character and importance of pyridazine, pyrazine, benzimidazole, benzoxazole, 1,2,3-triazines, tetrazole, 1,3,4-thiadiazole, tetrazines and pteridines.	**8**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Title/ Publisher	Year of Publication
1.	Katritzky A.R. and Pozharskii A.F., "Handbook of Heterocyclic Chemistry", 2nd Ed.,Pergamon,	**2000**
2.	Mann J. "Secondary metabolism", Oxford Chemistry Series.	**1987**
3.	Apsimon, J., "Total Synthesis of Natural Products", Vol. 1-5, Wiley.	**2013**
4.	Warren S. "Organic synthesis-The disconnection approach", Wiley.	**2008**
5.	Nicolaou K.C. and Sorenson, E.J., "Classics in Total Synthesis", Wiley.	**1996**
6.	Anasta, P.T. and Warner, J.C. "Green Chemistry: Theory and Practical", OUP, USA	**2000**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject code: **CYN-731** Course Title: **Characterization Techniques**
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 impart knowledge on characterization techniques used in industries and for R&D.
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**X-Ray**: Concept of X-ray spectra; detection of X-ray; absorption methods- absorption law, absorption edge analysis; X-ray emission spectroscopy – direct method, X-ray fluorescence method, energy dispersive and wavelength dispersive method; X-ray diffraction- concept of lattice, space groups, crystalline state, types of crystal system, scattering of X-ray, amplitude and phase of diffraction, structure factors, experimentation – powder method, indexing, unit cell parameters, characterization of crystalline materials; single crystal method, interpretation of diffraction data, calculation of structure factor, electron density maps and structure determination, R-factors and applications.	**10**
2.	**Surface Characterization**: X-ray photoelectron spectroscopy – chemical shift, instrumentation, qualitative and quantitative analysis, electron spectroscopy for chemical analysis, scanning electron microscopy – principle of electron matter interaction, instrumentation and use of energy dispersive x-ray analysis; transmission electron microscopy – reciprocal space and lattice, Ewald sphere, diffraction from crystal, bright and dark field imaging, indexing of diffraction pattern; Auger electron spectroscopy; Atomic force microscopy – concepts and instrumentation; Scanning probe microscopy – concepts and instrumentation.	**9**
3.	**Thermal Method**: Instrumentation on thermogravimetric analysis (TGA); differential thermal analysis (DTA); differential scanning calorimeter (DSC); use of thermal methods for characterization of materials.	**4**
4.	**Mass spectroscopy**: Instrumentation, types of ion sources, mass analyzers, resolution, nitrogen rule, ring rule, McLafferty's rearrangement, interpretation of mass spectrum, hyphenated techniques (GC-MS and LC-MS).	**7**
5.	**Nuclear magnetic resonance**: Instrumentation, FT-NMR spectrometer, chemical shift, spin-spin coupling, spin- spin decoupling, ^{1}H and ^{1}-C-NMR, and 2D-NMR, data interpretation, Zeugmatography and biological applications.	**7**
6.	**EPR Spectroscopy**: Principle and instrumentation, g-values and hyperfine coupling, spin densities and McConnell relation, interpretation of organic radicals; spectra of inorganic complexes, zero field splitting and Krammers degeneracy, anisotropy in the hyperfine coupling constant, single crystal EPR nuclear quadrupole interaction, spectral interpretation of transition metal complexes; general introduction to double resonance experiments, ENDOR, ELDOR, biological applications.	**5**
	Total	**42**

11. Suggested Books:

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

	Hill.	
2.	Skoog D.A., West D.M., Holler F.J. and Crouch S.R., "Fundamentals of Analytical Chemistry" 8th Ed., Thomson Brooks/Cole.	**2004**
3.	West A.R., " Solid State Chemistry and its Applications", John Wiley & Sons.	**2002**
4.	Williams D.B. and carter C.B., "Transmission Electron Microscopy: A Textbook for Materials Science, 2nd Ed., Springer.	**2003**
5.	Goldstein J., Newbury D.E., Joy D.C., Lyman C.E., Echlin P., Lifshin E., Sawyer L and Michael J.R., "Scanning Electron Microscopy and X-Ray Microanalysis", 3rd Ed., Springer 2003.	**2003**
6.	Parish R.V., "NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Spectroscopy", 1st Ed, Ellis Horwood Limited.	**1990**
7.	Banwell C.N. and Mc Cash E.M., "Fundamentals of Molecular Spectroscopy" 4th Ed., 1998, 30th reprint, Tata Mc Graw Hill.	**2008**
8.	Drago R.S., "Physical Methods for Chemists" 2nd Ed, Saunders College Publishing.	**1992**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-732** Course Title: **Environmental Chemistry**

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

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

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

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

8. Pre-requisite**: Nil**

9. Objective: To provide knowledge of environment chemistry.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Chemistry and the Environment:** Environment segments, ecosystem and natural cycles of the environment, chemical and photochemical reactions in the atmosphere, ozone chemistry, oxides of sulphur and nitrogen, organic compounds, green house effect and global warming, acid rain, environmental fate of pollutants, biological activity, biodegradation of carbohydrates, fats and oil, proteins, detergents, pesticides.	**9**
2.	**Chemical Toxicology:** Toxic chemicals in the environment, toxic effects, biochemical effects of arsenic, cadmium, lead, mercury, copper, chromium; biochemical effects of some gaseous pollutants, cyanide, pesticides, asbestos.	**6**
3.	**Pollution:** Air pollutants, air quality standards, sampling and analysis, air pollution control, noise pollution, injurious effects of noise.	**3**
4.	**Water Quality:** Water quality parameters and standards, turbidity, color, pH, acidity, solids, hardness, chlorides, residual chlorine, sulfates, fluorides, phosphates, iron, manganese, nitrogen, DO, BOD, COD, grease, volatile acids, analytical techniques in water analysis, soil pollution.	**9**
5.	**Wastewater Treatment:** Primary treatment, equalization, neutralization, proportioning, sedimentation, oil stripping of volatile organic, biological treatment process, lagoons, activated sludge process, trickling filtration, anaerobic decomposition, sludge handling and treatment process.	**9**
6.	**Adsorption and Oxidation Processes:** Theory of adsorption, ion exchange process, chemical oxidation, advanced oxidation process, miscellaneous treatment processes.	**6**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/ Reprint
1.	De A.K., "Environmental Chemistry", 7th Ed. New Age International (P) Ltd.	**2010**
2.	Sawyer C.N., "Chemistry for Environmental Engineering", 4th Ed., McGraw, Inc.	**1994**
3.	Metcalf E., "Wastewater Engineering", 3rd Ed., McGraw Hill Inc.	**1991**
4.	Manahan S.E., "Environmental Chemistry", 8th Ed., CRC Press.	**2005**
5.	Masters G.M., "Introduction to Environmental Engineering and Science", Prentice Hall of India Pvt. Ltd.	**1998**
6.	Khopkar S.M., "Environmental Pollution Analysis", New Age International (P) Ltd.	**2008**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-741** Course Title: **Chemometrics and Modelling**
2. Contact Hours: **L: 3** **T: 0** **P: 2**

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

4. Relative Weight**: CWS 15 PRS 25 MTE 20 ETE 40 PRE 0**

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

8. Pre-requisite**: Nil**

9. Objective: To import knowledge of modern methods of reducing and analyzing chemical data.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Fundamentals, probability and statistics:** Representation of simultaneous equations in matrix form, scalars, vectors and matrices; The matrix inverse, eigen values and eigenvectors, false negatives, false positives and power in testing of means; Regression (linear and nonlinear regression, curve fitting of chemical models, chemical calibration to concentration and properties, signal processing (digital filters, derivative filters, noise, Fourier transforms).	**14**
2.	**Treatment of Data*:*** Sources of error, precision and accuracy, propagation of errors (random errors, systematic errors, correlated errors), distributions (binomial distribution, sampling of solids, Poisson distribution, shot noise, gaussian distribution, chi-squared distribution, Student t- distribution, confidence intervals), hypothesis testing (t-test, types of errors, paired t-test, F-test, chi-squared test, Q-test), simple analysis of variance and experimental design (one-way, two-way with and without replicates, randomized and blocked designs).	**14**
3.	**Computational methods:** Introduction to digital computers, representation of numbers, errors in floating point representation; Algorithms, syntax of one higher level language suitable for scientific computations (C or Fortran)- declarations, assignment statement, input/output statements, control structures for selection and iteration, functions, array data structure, selected numerical methods for data analysis and treatment, writing and implementation of simple programs and one individually assigned programming project.	**14**
	Total	**42**

List of Practicals:

1. Writing C program using input and output statements.
2. Writing C program to demonstrate the concept of scope of variables.
3. Writing C program involving functions.
4. C program for analysis of errors.
5. C program for least square analysis.
6. Geometry optimization of small molecules using Gaussian 09 program.
7. Calculation of IR frequencies of sample using Gaussian 09 program.
8. Computation of excitation energies for small molecules using Gaussian 09 program.
9. Conformational analysis using molecular modeling.
10. C programming projects involving chemical calculations.

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/ Reprint
1.	Balagurusamy E., "Programming in ANSIC", Tata McGraw-Hill.	**2004**
2.	Anderson R.L., "Practical Statistics for Analytical Chemists", John Wiley.	**1970**
3.	Brereton R.G., "Applied Chemometrics for Scientists", John Wiley.	**2007**
4.	Goyal M., "Comprehensive Computer Based Numerical and Statistical Techniques", Laxmi Publications (P) Ltd.	**2006**
5.	Miller J.N. and Miller J.C., "Statistics and Chemometrics for Analytical Chemistry", Pearson Education Ltd.	**2005**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-742** Course Title: **Analysis of Materials**

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**: Spring** 7. Subject Area**: PEC**

8. Pre-requisite**: Nil**

9. Objective: To provide advanced knowledge of chemistry of engineering materials and their analysis.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Steel, Ferro and Non-Ferro Alloys:** Analysis of major constituents such as combined and uncombined carbon and silicon; Analysis of various metals present in steel, ferrochrome, ferromanganese, ferrovanadium, ferromolybdenum and ferrotungsten; Systematic determination of various metal ions in non-ferro alloys, analysis of major constituents in brasses, bronzes, gun metal and white metal.	**10**
2.	**Analysis of Constituents of Mortar and Concrete:** Classification of cements, various constituents of cement; Analysis of Portland cement with reference to insoluble residue, total silica, sesquioxides, iron, lime and manganese.	**6**
3.	**Analysis of Paints:** Identification of thinner, vehicle and their analysis, classification of pigments, analysis of various constituents in different pigments, varnishes, catalyzed coating and metal manganese.	**6**
4.	**Oils, Lubricants and Greases:** Testing of lubricating and allied oils with reference to viscosity and viscosity index, cloud and pour points, flash and fire points, aniline points, neutralization number, total acid number, Koettsdoerfer number and iodine value; Mechanical stability of greases, determination of penetration number and dropping point of grease, analysis and characterization of petroleum products.	**10**
5.	**Detergents:** Various constituents of detergents, quantitative analysis of anionic, cationic, amphoteric, ampholytic and zwitterionic surfactants; Determination and identification of major organic components such as sodium carboxymethyl cellulose, NTA, EDTA, organic bleaches and inorganic constituents; Analysis of soap products.	**10**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/ Reprint
1.	Agarwal B.C. and Jain S.P., "Metallurgical Analysis", Khanna Publications.	**1996**
2.	Virmani O.P. and Narula A.K., "Applied Chemistry: Theory and Practice", New Age International Publishers.	**2001**
3.	Longman G.F. "The Analysis of Detergents and Detergent Products", John Wiley & Sons.	**2000**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-751** Course Title: **Analysis of Industrial Polymers**

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**: PEC**

8. Pre-requisite**: Nil**

9. Objective: To provide knowledge of polymer chemistry and analysis of industrial polymers.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Introduction of Polymers:** Classification of polymers, homopolymers, copolymers, graft copolymers and their characteristic properties in reference to technological and industrial applications.	**6**
2.	**Thermal and Spectral Methods of Analysis of Polymers:** Applications of DSC, DTA, TG methods for analysis of homopolymers, copolymers, polymer blends and composites; Application of IR , NMR, X-ray diffraction neutron scattering, SEM and TEM techniques for analysis of polymers; Viscosimetry for the analysis of molecular mass and molecular dimension of polymer coils.	**12**
3.	**Mechanical Behavior of Polymers:** Analysis of mechanical properties such as tensile, polymers shear and flexural strengths.	**6**
4.	**Polymers for Advance Technologies:** Testing of polymers for electrical and electronic applications; Analysis of optical properties of polymers in presence of coloring agents, effects of radiation on stability of polymers.	**6**
5.	**Reinforced and Multi-component Polymers:** Analysis of fillers, antioxidants, stabilizers, plasticizers, fire retardants, pigments and other additives in industrial polymers using modern methods of analysis.	**6**
6.	**Commercial and Industrial Polymers:** Polymer liquid crystals, polymeric foams, polymer blends, thermosets and thermoplasts, biodegradable polymers, ion exchangers, engineering plastics and conducting polymers.	**6**
		42

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/Reprint
1.	Billmeyer Jr. F.W., "Text Book of Polymer Science", 3rd Ed., Wiley-Interscience.	**1994**
2.	Fried J.R., "Polymer Science and Technology", Prentice-Hall.	**2002**
3.	Seymeur R.B. and Carraher Jr. C.E., "Polymer Chemistry", Marcel Dekker.	**1981**
4.	Dyson R.N., "Specialty Polymer", Chapman and Hall.	**1987**
5.	Ku C.C., Liepins R., "Electrical Properties of Polymers", Hanser Publications.	**1987**
6.	Morgoles J M., "Conducting Polymers and Plastics", Chapman-Hall.	**1989**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-752** Course Title: **Analysis of Food and Drugs**

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**: Spring** 7. Subject Area**: PEC**

8. Pre-requisite**: Nil**

9. Objective: To provide knowledge of composition and analysis of foods and drugs.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Analysis of Basic Constituents of Food:** Moisture in case of dry, wet, moist food, oils, fats and fat emulsions in case of fatty foods, volatile oil in case of spices, fibre determination in fibre containin food such as cereal, bread, spices (to determine quality of spices), protein in all kinds of food; Ash determination of sulfated ash, water soluble ash and siliceous matter in vegetables, spices, sugars in fru juices and soft drinks, acidity and volatile acidity, pH value.	**10**
2.	**Analysis of Preservatives, Colouring Matter and Contaminants:** Determination of SO_2, benzoic acid, hydroxyl benzoates, nitrites, nitrates used as preservatives; Analysis of anti-oxidants in fats, such as BHT, BHA and gallates, coloring matter in soft drinks, alcoholic drinks, jam-jelly, sweets, contaminants- analysis of mercury, arsenic and trace elements.	**8**
3.	**Analysis of Drugs and Pharmaceuticals:** General pharmacology, qualitative aspects of drug action, receptors, role of absorption of drugs, routes for administration and elimination of drugs, gram positive and gram negative bacteria, 5-HT receptors and drugs action on 5-HT, non steroidal anti-inflammatory drugs; Analysis of chloramphenicol, chloroquine, phosphate, beta-methasone, amylobarbitone, analgin, ampicilline, ascorbic acid, aspirin and paracetamol.	**14**
4.	**Forensic Analysis of Common Poisons:** Poisoning due to arsenic, lead, cadmium, mercury and cyanide, general analytical approach; Case studies- death due to fire, explosions, drug overdose case; Alcohol- effects of alcohol, analysis of body fluid samples for alcohol, analysis of breath for alcohol; Analysis of body fluids- biological evidence, blood analysis, DNA analysis.	**10**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/Reprint
1.	Pearson D., "Lab Techniques in Food Analysis", Butter Worth and Co. Ltd.	**2003**
2.	Mayer L.H., "Food Chemistry", The AVI Publishing Co.	**2005**
3.	Mac Leod A.J., "Instrumental Methods of Food Analysis", Elec Science.	**1975**
4.	ISI Handbook of Food Analysis. Indian Standards Institution.	**2000**
5.	Rang H.P., Dale M.M. and Ritter J.M., "Pharmacology", Churchill Livingstone.	**1996**
6.	George C, Thomas M and Pearmain H, "Aids to the Analysis of Foods and Drugs", 4th Ed., Bibliobazar, LLC, Bibliolife.	**2003**
7.	Pearmain T.H. and Moor C.G., "The Analysis of Foods and Drugs", Balliere, Tindall and Cox.	**2007**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-762** Course Title: **Drug Design and Action**

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**: Spring** 7. Subject Area**: PEC**

8. Pre-requisite**: Nil**

9. Objective: To provide knowledge of the design of drugs and their mode of action.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Drug Design Concepts**: Stereochemistry, formation of salts, solubility of drugs, importance of water solubility, structure activity relationships (SARs), quantitative structure activity relationships (QSARs), liphophilicity and stereo-electronic effects; Computer aided design and combinatorial methods, encoding methods, combinatorial synthesis in solution, screening and deconvolution.	**10**
2.	**Drugs and Their Action:** Sources of drugs, classification of drugs, routes of administration, pharmaceutical phase, pharmacokinetic phase, bioavailability of a drug and pharmacodynamic phase.	**4**
3.	**Examples of Drug Action:** Concept of antibiotics, membranes-types, transport across membranes, drugs that disrupt membranes, enzymes-biological catalysis enzyme kinetics, enzyme inhibition, design of enzyme inhibitors, reversible inhibitors, transition state inhibitors, irreversible inhibitors; Receptors and messengers – types, ligand responses, ligand-receptor interactions, binding affinity, designing receptor based drugs-agonists and antagonists; Drugs that target nucleic acids, nucleic acid synthesis, inhibitors.	**14**
4.	**Drug Metabolism**: Phase I and phase II metabolic reactions.	**2**
5.	**Drug Synthesis**: Importance of chiral drugs, asymmetry in synthesis –creation of stereospecific centers, methods of asymmetric synthesis and disconnection approach, enantiomeric separation and characterization methods, drugs based on steroid, non-steroid, substituted benzene ring, five and six membered heterocycles.	**12**
	Total	**42**

11. Suggested Books:

S. No.	Authors/ Book/ Publisher	Year of Publication/Reprint
1.	Thomas G., "Fundamentals of Medicinal Chemistry", John Wiley and Sons.	**2003**
2.	Lednicer D., "Strategies for Organic Drug Synthesis and Design", Wiley-Interscience, John Wiley and Sons.	**1988**
3.	Dugas H., "Bio Organic Chemistry, A.Chemical approach to enzyme action", 2nd Ed., Springer – Verlag.	**1989**
4.	Roth H.J. Kleemann A., "Pharmaceutical chemistry", Vol.1, Drug Synthesis.	**2001**
5.	Berger A., "Medicinal chemistry", Vol. 1 and 2, Wiley Interscience.	**1990**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: **Department of Chemistry**

1. Subject Code: **CYN-772** Course Title: **Nuclear Techniques for Analysis and Characterisation**

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**: Spring** 7. Subject Area**: PEC**

8. Pre-requisite**: Nil**

9. Objective: To impart in-depth knowledge on nuclear techniques for analysis and characterization of materials.

10. Details of Course:

Sl. No.	Contents	Contact Hours
1.	**Basic Radiochemistry:** Types of radioactivity, decay methods, radioactive equilibrium, choice and production of radio nuclides, interaction of radiation with matter.	6
2.	**Nuclear Detector:** Properties of a detector, gas filled counters, scintillation and semiconductor detectors, clover detectors.	4
3.	**Applications of Radioactivity:** Isotope dilution analysis, radioimmunoassay, radiochemical methods for determining biological activity, radiopharmaceutical, neutron activation analysis.	8
4.	**Ion Beam Analysis and Micro-analysis:** Proton Induced X-ray Emission (PIXE), Rutherford Backscattering Spectrometry (RBS), nuclear reactions analysis. Nuclear Microprobe- μ-PIXE, μ-RBS, scanning transmission ion microscopy (STIM); Comparison with other microprobes- electron microprobe, synchrotron based μ-XRF	10
5.	**Applications of Ion Beam Analysis:** Quantitative elemental imaging, applications to biomedical science, geological science, materials science, toxicology, single cell irradiation, proton beam writing for nanostructure fabrications.	14
	Total	42

11. Recommended Books:

S. No	Authors/Book/Publisher	Year of Publication/ Reprint
1.	Ehmann W.D. and Vance D.E., "Radiochemistry and Nuclear Methods of Analysis", John Wiley and Sons.	1991
2.	Sood, D.D., Reddy A.V.R. and Ramamoorthy N., "Fundamentals of Radiochemistry" Indian Association of Nuclear Chemists and Allied Scientists.	2004
3.	Johansson S.A.E., Campbell J.L. and Malmqvist K.G. (Eds), "Particle Induced X-Ray Emission Spectrometry, (Chemical Analysis: A series of monographs on Analytical Chemistry and Applications)", Wiley Interscience.	1995
4.	Meyer J.W. and Rimini, E., "Ion Beam Handbook for Material Analysis" Academic Press.	1987

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject code: **CYN-782** Course Title: **Chemistry of Industrial Processes**
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: **Spring** 7. Subject Area: **PEC**
8. Pre-requisite: Nil
9. Objective: To impart knowledge on different types of synthesis processes in industries and R&D
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Chemicals and processes in petroleum industries.** Petroleum distillation, shale gas, naphtha versus gaseous feed stocks, heavier oil fractions, steam cracking and petroleum refining reactions, catalytic cracking, mechanisms of steam and catalytic cracking, catalytic reforming, oligomerization, alkylation, hydrotreating and coking, dehydrogenation, isomerization, metathesis, chemicals and polymers from ethylene, propylene, C4 stream, C5 stream, benzene, toluene, xylenes, synthesis gas and coal.	**14**
2.	**Catalysis and green chemistry**. Importance and role of catalysts, catalyst choice, homogeneous and heterogeneous catalysis, catalysts promoters, catalysts poisoning, catalysis by acids and bases, dual function catalysis, catalysis by metals and metal oxides, semiconductors, and insulators, coordination catalysis, enzyme, shape-selective catalysts, phase-transfer and fluorous biphase catalysis, nanocatalysis, photocatalysts, green chemical methods, green solvents and green pharmaceuticals.	**14**
3.	**Industrial Processes:** oxidation, hydrogenations, isomerization reactions, synthetic route to menthol, carbonylations, water-gas shift reaction, hydroformylation, Fischer-Tropsch reaction, carbon-carbon bond forming reactions, alkylations, activation of aryl and vinyl halides, fine chemicals, metathesis of olefins, polymerization reactions, Ziegler-Natta catalysts, Phillips catalysts, metal-carbene, Schrock carbenes and Fischer carbenes.	**14**
	Total	**42**

11. Suggested Books:

S. No.	Name of Authors/Book/ Publisher etc.	Year of Publication/ Reprint
1.	Chiusoli G.P. and Maitlis P.M. " Metal-catalysis in Industrial Organic Processes, Editor: RSC publishing,	**2007**
2.	Dunn, P.J., Wells, A. and Williams, M.T. "Green Chemistry in the Pharmaceutical Industry", Wiley-VCH,	**2010**
3.	Wittcoff, H.A., Reuben, B.G. and Plotkin, J.S. "Industrial Organic Chemicals" 3rd Ed., Wiley-VCH	**2013**