INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-301 Course Title: **Quantum Chemistry and Chemical Bonding**
2. Contact Hours: **L: 3** **T: 1** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 4** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Fundamental knowledge in physical chemistry
9. Objective: To introduce the formalism, mathematical treatment and applications of quantum mechanics relevant to chemistry problems

10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Quantum Chemistry:** Separation of variables, power series solution of differential equations, Harmonic oscillator - classical and quantum mechanical treatment, wave functions and energy levels; particle in a ring and a sphere, spherical polar coordinates, angular momentum, Legendre and associated Legendre functions, spherical harmonics, Hydrogenic systems, separation of θ, φ and R-equations, solving the radial equations, radial functions, quantum states, Zeeman effect.	**12**
2.	**Many Electron Systems:** Electron spin, spin orbitals, symmetric and antisymmetric wave functions, Slater determinants for ground and excited states of small species, Hamiltonian for many electron systems, self-consistent field theory; Hartree and Hartree-Fock methods, spin-orbit interaction, Term symbols for atoms	**10**
3.	**Approximation Methods:** Need for approximations methods**,** selection of trial function, variation theorem, linear and nonlinear variation functions, perturbation methods, perturbation parameter, first, second and higher order corrections to wave functions and energies, use of approximation methods to various systems.	**8**
4.	**Chemical Bonding:** Born-Oppenheimer approximation, nuclear motion in diatomic molecules, bonding in H_2^+ and H_2, molecular orbital and valence bond theory treatments, homo and hetero nuclear diatomic molecules, poly atomic molecules, Virial theorem and Hellmann-Feynmann theorem, Hückel molecular orbital theory-applications to π-electron systems; Hybridisation-sp, sp^2, sp^3 mathematical treatment, semi-empirical and *ab initio* methods.	**12**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Levine, I. N., "Quantum Chemistry", 5th Edition, Pearson Education	**2000**
2.	McQuarrie, D. A., "Quantum Chemistry", Student Edition, Viva Books	**2011**
3.	Atkins, P. W., "Molecular Quantum Mechanics", 4th Ed., Oxford University Press	**2010**
4.	Engel, T., "Quantum Chemistry and Spectroscopy", 3rd Edition, Pearson	**2012**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-303 Course Title: **Advanced Coordination Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Fundamental knowledge in coordination chemistry and organometallics
9. Objective: To impart advanced concepts of transition metal chemistry.
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Stereochemistry of Coordination Compounds**: 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).	4
2.	**Molecular Orbital Theory of Coordination Compounds:** Introduction to character table and symbols, construction of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ- and π-bonding; angular overlap model.	**7**
3.	**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, ligand field parameters; fluorescent and phosphorescent complexes.	**8**
4.	**Molecular Magnetism and Magnetic Properties of Coordination Compounds:** Magnetic susceptibility and magnetic moment; molecular magnetism - 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 crossover 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, single molecular magnets.	**14**
5.	**Photochemistry of Coordination Compounds**: Introduction to inorganic photochemistry, photochemically excited states and excited state processes for transition metal complexes, types of photochemical reactions of coordination compounds–substitution, decomposition, fragmentation, rearrangement and redox reactions. Unimolecular charge-transfer photochemistry of cobalt (III) complexes. Mechanism ofligand to metal charge transfer photoreduction. Ligand-field photochemistry of Cr(III) complexes, Adamson's rules, photoactive excited states, Vincenzo-*Carassiti* model – photophysics and photochemistry of ruthenium polypyridyl complexes, emission and redox properties and Reinecke's salt as a chemical actinometer.	**9**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Douglas B.E., McDaniel D.H. and Alexander J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons.	**2001**
2.	Purcell, K.F., Kotz, J.C., "Inorganic Chemistry", Saunders, London,	**1977**
3.	Figgis, B.N. and Hitchman, M. A "Ligand Field Theory and Its Applications"	**1999**
4.	Huheey, J.E.,Keiter, E.A., Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity" 4th Ed, Pearson Education, Inc.	**2003**
5.	Adamson, A.W. "Inorganic Photochemistry", Wiley, New York.	**1975**
6.	Roundhill, D.M. "Photochemistry and Photophysics of Metal Complexes", Springer, New York.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-305 Course Title: **Organic Chemistry III**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Fundamental knowledge in organic chemistry
9. Objective: To impart knowledge of stereochemistry and reaction mechanism in Organic Chemistry
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Stereochemistry:** Basic Dynamic stereochemistry: Conformation and Reactivity. Various chemo, region and stereoselective reactions.	**5**
2.	**Reactive Intermediates:** Carbenes and carbenoids; structure, reactivity, selectivity and mechanisms of radicals and radical based reactions involving various functional groups; radical cations and radical anions; Nonclassical carbocation; sigma and pi-participation.	**9**
3.	**Mechanistic and Stereochemical Aspects:** Baeyer-Villiger, Claisen (including Johnson-Claisen, Ireland-Claisen, Eschenomser, Overman modifications) Cope, oxy-Cope and Wittig rearrangements; ene and metalloene reactions; (2+2), (3+2) and (4+2) cycloadditions; Barton reaction.	**11**
4.	**Organometallics in organic synthesis:** Mechanism and stereochemistry of metal catalyzed organic transformations: Palladium- catalyzed reactions such as Heck, Stille, Suzuki, Sonogashira, Kumada, Negishi, Buchwald-Hartwig couplings; Tsuji-Trostreaction; Cr-catalyzed reactions.	**9**
5.	**Enzymatic Reactions:** Mechanistic and stereochemical aspects of hydrolases (including esterases and lipases), oxidoreductases.	**4**
6.	**Green Chemistry:** Twelve principles, examples, sustainability and advantages for organic reactions, aqueous organometallic reactions.	**4**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Smith, M.B., "March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure", 7th Edition John Wiley & Sons, Inc.	**2013**
2.	Carey, Francis A., Sundberg**,** Richard J., "Advanced Organic Chemistry Part A: Structure and Mechanisms" 5th Edition Springer	**2007**
3.	Carey, Francis A., Sundberg**,** Richard J., "Advanced Organic Chemistry Part B: Structure and Mechanisms", 5th Edition, Springer	**2007**

4.	Clayden, J., Greeves N. Warren S., "Organic Chemistry Second Edition", Oxford University Press.	**2015**
5.	Carruthers W., Coldham I., "Modern Methods of Organic Synthesis South Asia Edition", Cambridge University Press.	**2015**
6.	Sykes, P.A., "Guidebook to Mechanism in Organic Chemistry", 6th Edition, John Wiley & Sons, New York.	**2013**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-311 Course Title: **Laboratory 1**
2. Contact Hours: **L: 0** **T: 0** **P: 12**
3. Examination Duration (Hrs.): **Theory 0** **Practical 6**
4. Relative Weightage**: CWS 0** **PRS 50** **MTE 0** **ETE 0** **PRE 50**
5. Credits**: 6** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Basic concepts in chemistry
9. Objective: To provide knowledge laboratory based experiments
10. Details of the Course:

Physical Chemistry:

1. Determination of pK_1 and pK_2 of dibasic acids.
2. Determination of cell constant and verification of Kohlrausch's law.
3. Determination of specific rotation and molar rotation of lactic acid/sucrose by polarimetry.
4. Determination of molar refraction equivalent of $-CH_2$, C, H, and O.
5. Determination of composition of liquid mixture by refractive index measurements.
6. Determination of dimerization constant of benzoic acid.
7. Conductometric titration of different acids against bases
8. Determination of surface excess concentration and thickness of interfacial adsorbed layer by surface tension measurements of water-n-butanol mixture using capillary rise method
9. Determination of the Parachor of binary mixture of miscible solutes by surface tension measurements.
10. Verification of Hardy-Schulze rule for positive/negatively charged colloids.
11. Determination of critical micelle concentration of sodium dodecylsulphate/cetyltri-methylammonium bromide by surface tension method.
12. Determination of λ_{max} of compounds by UV-Vis spectroscopy
13. Measurement of viscosity of solutions of a polymer and calculation of its average molecular weight.
14. Study of oscillatory reactions.

Inorganic Chemistry

1. Semi-micro qualitative analysis involving six/eight radicals with interfering radicals
2. Following experiments are based on volumetric method :
   a) Determination of Cr(III) volumetrically.
   b) Determination of Fe(III) volumetrically.
   c) Determination of Cu(II) and Zn(II) in a mixture. (two experiments)
   d) Determination of Mn(II) and Fe(III) in a mixture.
   e) Determination Ni(II) and Fe(III) in a mixture.
   f) Determination of Cu(II) and Ni(II) in a mixture.
   g) Determination of chloride content in water samples by Mohr's/ Volhard's method/ by use of tetrazine as indicator.
   h) Iodo and iodimetric titrations for estimation of Cu, Fe and Mn salts.

Organic Chemistry

1. Qualitative analysis: Identification of binary mixtures of organic compounds through TLC, crystallization, melting point, derivatisation, and IR spectroscopy (3 turns)
2. Estimations of organic functional groups in (i) glucose and (ii) phenol (2 turns)
3. Separation of binary mixture by column chromatography.
4. Kinetic and thermodynamic control of reactions: Semicarbazone formation of cyclohexanone and 2-furfuraldehyde in different buffers
5. Kinetics of solvolysis of 2-chloro-2-methylbutane (2 turns)
6. The aldol condensation: Synthesis of dibenzalacetone
7. Oxidation of benzoin to benzil
8. Reduction of benzil to hydrobenzoin
9. Bromination of acetanilide nitration of bromobenzene

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-302 Course Title: **Group Theory and Spectroscopy**
2. Contact Hours: **L: 3** **T: 1** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 4** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Fundamental knowledge in physical chemistry
9. Objective: To provide knowledge on molecular symmetry and spectroscopy
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Molecular symmetry:** Symmetry elements and symmetry operations, groups mathematical and molecular groups, Abelian, cyclic and polymorphic groups, identification of molecular point groups, subgroups, group multiplication table, classes.	**6**
2.	**Representation of groups:** Matrix representation of various symmetry operations, reducible representation, basis, great orthogonality theorem and its consequences, irreducible representation, construction of character table, representation of cyclic groups.	**8**
3.	**Applications of Group theory:** Direct product, vanishing and non-vanishing integrals, spectral transition probabilities, electronic transitions, symmetry of normal modes of vibrations, prediction of infrared and Raman active modes,orbital overlap, symmetry adapted linear combinations, projection operator.	**7**
4.	**Microwave spectroscopy:** Classification of rotors, population of energy levels and intensity of rotational lines, anharmonicity and centrifugal distortion, effect of isotopic substitution, rotational spectra of linear, spherical top and asymmetric top polyatomic molecules, instrumentation.	**7**
5.	**Infrared and Raman spectroscopy:** Vibration of polyatomic molecules, harmonic and anharmonic oscillators, types of vibration bands-overtones, combination bands, Fermiresonance, finger print region, FT-IR spectroscopy and applications, Raman Spectroscopy- Rayleigh and Raman scattering, polarisabilities, rotational and vibrational Raman spectra, selection rules, laser Raman spectroscopy.	**5**
6.	**UV-visible spectroscopy:** Electronic spectra, Franck-Condon principle, pre-dissociation spectra, Fortrat diagram, electronic spectra of organic compounds, types of transitions, solvent effects, Woodward Fieser rule for prediction of λ_{max} in conjugated polyenes and enones, electronic transition in inorganic complexes, charge transfer spectra of organic and inorganic compounds.	**4**
7.	**Photoelectron spectroscopy:** Ionization process, Koopman's theorem, spectrum of core electron, spectrum of some specific cases like dinitrogen, dioxygen, hydrogen fluoride, spin-orbit coupling, X-ray photoelectron spectroscopy, zero kinetic energy spectroscopy, Auger electron spectroscopy, electron energy loss spectroscopy with examples.	**5**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Ladd, M., "Symmetry and Group Theory in Chemistry", Horwood publishing,	**2000**
2.	Cotton, F.A., "Chemical Applications of Group Theory", 3rd Edition, Wiley	**2008**
3.	Banwell, C.N. and McCash, E. L. M., "Fundamentals of Molecular Spectroscopy", 4th Edition, McGraw Hill, N. Y.	**2017**
4.	Graybeal, J.D., "Molecular Spectroscopy", 1st Rev. Edn, McGraw-Hill	**2014**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-304 Course Title: **Solid State Chemistry and Applications**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Spring** 7. Subject Area**: PCC**
8. Pre-requisite**:** Fundamental concepts in physical and inorganic chemistry
9. Objective: To provide knowledge on crystal symmetry, structure, bonding and properties of solids

10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Descriptive crystal chemistry and crystal defects:** Binary and ternarysolid compositions and some important structure types: AB- rock-salt, CsCl, zinc blende, wurtzite, NiAs; AB_2- fluorite, rutile, antifluorite, $CdCl_2$, CdI_2; ABX_2- ordered and disordered rock-salt, delafossite; AX_3- ReO_3 and skutterudite; ABX_3- perovskite, ilmenite, tunnel structures, AB_2X_4/A_2BX_4- spinel, K_2NiF_4; $A_2B_2O_7$-pyrochlore, layered oxides; $A_3B_2(SiO_4)_3$-garnets. Imperfections in solids- point and extended defects, non-stoichiometric defects- vacancy and interstitial; stacking faults, dislocations, CS planes and Wadsley defects; grain and anti-phase boundaries.	**10**
2.	**Geometrical crystallography:** Crystal habit and symmetry in the crystalline state, translational symmetry- screw axis and glide planes, symmetry in different crystal systems, point groups and their stereographic projections, space symmetry and space groups, Schoenflies and Hermann-Mauguin notations, Wyckoff symbols, general and special positions, representation of space groups and international table of crystallography.	**8**
3.	**Structure determination:** X-ray diffraction,quadraticform of the Bragg's law, concept of reciprocal space, Bragg's law in the reciprocal space, Ewald sphere construction, amplitude and phase of X-ray diffraction, structure factor and integrated intensity, crystal symmetry and systematic absences, indexing and identification of crystal systems.	**6**
4.	**Bonding in solids:** Bonding in molecular solids- polymorphism, bonding in extended solids- ionic, covalent and metallic; Band theory of solids- classification of insulators, semiconductors and metals, free electron theory, Bloch's theorem, concept of density of states and elementary band theory, band structures of one-, two- and three-dimensional solids.	**8**
5.	**Properties of solids:** Optical properties, electrical conductivity, mobility, thermal conductivity, specific heat, magnetic properties- magnetization, susceptibility, hysteresis, magnetic anisotropy, dielectric properties- paraelectric, pyroelectric, piezoelectric and ferroelectric	**6**

6.	**Physical methods for characterization of solids:** Thermal analysis; optical and electron microscopy; UV-visible and IR spectroscopy; X-ray spectroscopy; photoelectron spectroscopy, Mössbauer spectroscopy.	**4**
	Total	**42**

11. Suggested Books

Sl. No.	**Authors/ Title/ Publisher**	**Year of Publication/ Reprints**
1.	West, A.R., "Solid State Chemistry and its Applications", Reprint, Wiley India	**2013**
2.	Stout, G.H. and Jensen, L.H., "X-Ray Structure Determination: A Practical Guide", 2nd Edn., Wiley-Interscience	**1989**
3.	Giacovazzo, C., Artioli, G. and Monaco, H.L. "Fundamentals of Crystallography", Oxford University Press	**2006**
4.	Wells, A.F. "Structural Inorganic Chemistry", 5th Edn., Clarendon Press, Oxford	**1984**
5.	Spaldin, N., "Magnetic Materials: Fundamentals and Device Applications", Cambridge University Press	**2003**
6.	Sutton, A.P. and Sutton, A.D. "Electronic Structure of Materials", Oxford University Press	**1993**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-306 Course Title: **Organic Chemistry- IV**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Basic concepts in organic chemistry
9. Objective: To impart knowledge of structure and mechanism in Organic Chemistry
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Conformation in cyclic structures:** Conformations in cyclobutane, cyclopentane and cycloheptanes; Monosubstituted cyclohexanes: characteristics of chair form, ring inversion, flexible conformers and their stability, isolation and characterization of conformers; di- and polysubstituted cyclohexanes, normal and atypical disubstitutedcyclohexanes, twist boat conformers; cyclohexane ring with one or two sp^2 carbon atoms, alkylidenecyclohexanes, cyclohexenes; conformational analysis of four, five and six membered heterocycles, anomeric effect, rabbit ear effect; conformational effect on base-induced and pyrolytic eliminations, solvolysis, esterification, hydrolysis, oxidation, reduction. Fused ring systems- decalin, perhydroanthracene, perhydrophenanthrene and cyclopentanoperhydrophenanthrene, bicycloheptanes, norbornyl cation.	**12**
2.	**Heterocyclic chemistry:** Classification and naming of heterocyclic compounds, molecular orbital picture; characteristics of pyrrole, furan, thiophene and pyridine; methods of preparation (Paal-Knorr, Feist-Benary, Hantzsch and Knorr syntheses); electrophilic and nucleophilic substitution reactions in pyridines; five and six membered rings with two or more heteroatoms (thiazoles, isoxazoles, imidazoles, pyrazines) and their synthesis, basicity and reactivity; fused heterocyles -preparation and reactions of indoles, quinolines and isoquinolines (Fisher indole, Skraup, and Bischler-Napieralski syntheses); mechanism of electrophilic substitution reactions in indoles, quinolines and isoquinolines.	**11**
3.	**Pericyclic Reactions:** Woodward-Hoffmann description of the Diels-Alder reaction, trapping reactive intermediates by Diels-Alder reaction, other thermal cycloaddition reactions, 1,3-dipolar cycloadditions,ene reaction,sigmatropic rearrangement, orbital description and the direction of [3,3]-sigmatropic rearrangement, [2,3]-and [1,5]-sigmatropic rearrangements, electrocyclic reactions, Cope and aza-Cope rearrangements.	**11**
4.	**Disconnection approach:** 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**

	Total	**42**

11. Suggested Books

Sl. No.	**Authors/ Title/ Publisher**	**Year of Publication/ Reprints**
1.	Carey F.A. and Sundberg, R.J., "Advanced Organic Chemistry Part A: Structure and Mechanisms", 5th Edn, Springer Publishers	**2007**
2.	Clayden J., Geeves N. and Warren S., "Organic Chemistry", 2nd Edn, Oxford University Press	**2012**
3.	Eicher T. and Hauptmann S., "The Chemistry of Heterocycles", 2nd Edn, Wiley-VCH Veriag GmbH & Co. KGaA.	**2003**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-312 Course Title: **Laboratory II**
2. Contact Hours: **L: 0** **T: 0** **P: 12**
3. Examination Duration (Hrs.): **Theory 0** **Practical 6**
4. Relative Weightage**: CWS 0** **PRS 50** **MTE 0** **ETE 0** **PRE 50**
5. Credits**: 6** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Basic concepts in chemistry
9. Objective: To provide knowledge in laboratory based experiments
10. Details of the Course:

Physical Chemistry

1. To study the kinetics of H^+-catalysed hydrolysis of sucrose by polarimetry.
2. Verification of Freundlich and Langmuir adsorption isotherms.
3. Determination of the equilibrium constant for $KI + I_2 = KI_3$ reaction using partition method.
4. Determination of the fluorescence quantum yield of the given substance.
5. Verification of Ostwald's dilution law by conductometric measurements of acetic acid.
6. Analysis of a mixture of metal cations by electroanalytical methods.
7. Determination of cation concentrations in soil by flame photometry and MP-AES
8. To calculate the surface energy of given organic liquid from surface tension versus temperature relationship.
9. To determine the variation of miscibility of phenol in water with temperature and to find the critical solution temperature. Analysis of effect of impurity on the CST.
10. To determine ΔG, ΔH and ΔS for the reaction, $Zn(Hg) + 2AgCl = ZnCl_2(aq) + 2\ Ag\ (s)$ from e.m.f measurements.
11. To determine the ionization constant of bromophenol blue indicator by spectroscopy.

Inorganic Chemistry

1. Gravimetric determination of copper as cuprous thiocyanate.
2. Gravimetric determination of nickel as nickel dimethylglyoxime.
3. Determination of zinc as zinc ammonium phosphate in white metal decorative items.
4. Determination of magnesium as magnesium pyrophosphate in Mg ribbon.
5. Determination of iron as ferric oxide in folic acid/ iron tablets/ iron waste.
6. Estimation of metal ions by gravimetric-cum-volumetric analysis (2 components), e.g.,
   a) Ag(I) gravimetrically and Cu(II) volumetrically.
   a) Cu(II) gravimetrically and Zn(II) volumetrically.
   b) Cu(II) and Ni(II) gravimetrically.
   c) Cu(II), Ni(II) and Zn(II) gravimetrically
   d) Cu(II), Ni(II) and Mg(II)
7. Preparation of Metal complexes

Organic Chemistry

1. Nucleophilic Aromatic Substitution: Preparation of 2,4-dinitrophenylthiocyanate from 2,4-dinitrobromobenzene
2. Preparation of 1,4-di-t-butyl-2,5-dimethoxybenzene by Friedel-Crafts alkylation

3. Bromination of alkenes (trans-cinnamic acid or styrene) and subsequent dehydrohalogenation
4. Cannizaro reaction: Conversion of p-nitrobenzaldehyde into p-nitrobenzoic acid and *p*-nitrobenzyl alcohol.
5. Preparation of Orange II or para red and dyeing cloth
6. Sandmeyer reaction: preparation of 2-iodobenzoic acid
7. Synthesis of chalcone from an aromatic aldehyde and acetophenone
8. Henry reaction: Synthesis of ω-nitrostyrene from an aromatic aldehyde and nitromethane
9. Coumarin synthesis from salicylaldehyde and diethylmalonate
10. Diels-Alder reaction of anthracene with maleic anhydride
11. Conversion of benzil to quinoxaline
12. Green synthesis of binaphthol
13. Preparation of *p*-nitroaniline from acetanilide (2 turns)

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-515 Course Title: **Art of Scientific/Technical Writing**
2. Contact Hours: **L: 2** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 2** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 2** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Basic chemistry knowledge
9. Objective: To introduce research ethics and methodologies for scientific writing in Chemistry
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1	**Information and resources:** Sources and their authenticity, methods for collecting information- search Engines, Google scholar, Scifinder, Web of Science, Scopus; Features of Chemdraw and its uses; searching of chemical resources, reactions, reagents and their chemical and physical properties.	**6**
2	**Data collection:** Spectral data bases, NMR data bases, CCDC, PDB, JCPDS, NIST. Recording of experiments: Log book and lab notebook, accuracy, precision, fitting of data, error bar, noise and data, IUPAC guidelines of presentation of data for experimental and theoretical studies. Figures, legends, tables, foot notes, abbreviations, references, different software used for plotting. Typesetting, templates, formulas and equations, reference formats, supplementary data	**5**
3	**Writing style:** Abstract, report, dissertation, thesis, manuscript, monographs, books, research proposals. Types of publications: letters, communications, perspectives, research articles, reviews, accounts. Outline, drafting, refinement, common errors, editing services, proof reading	**8**
4	**Ethics in research and publishing:** Authorship, plagiarism, checking of plagiarism, duplicate and redundant publications, copyright, open access licenses, embargo period, and repositories. Conflicts of interest, Bio-ethics. Social networks for promotion. Review, Originality, physical insights, reproducibility, Renowned publishers in the field of chemistry, citations, impact factor, Ranking: journals, institutes (e.g. NIRF), individuals, h-index, i-index, i-10 index, Author identification: ORCID and RESEARCHER IDs, ISSN and ISBN, Intellectual property rights	**7**
5	**Presentation:** Different modes: board, poster, power-point, audio-visual.	**2**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Hoffman, A., "Scientific Writing and Communication", Oxford University Press, 2nd Edn.	2014
2.	Katz, M. J., "From Research to Manuscripts: A Guide to Scientific Research", Springer, 2nd Edn.	2009
3.	Ebel, H. F., Bliefert, C., and Russey, W. E., "The Art of Scientific Writing", Wiley-VCH, 2nd Edn.	2004

4.	Tufte, E. R., “The Visual Display of Quantitative information”, Graphics Press, 2nd Edn	2001
5.	Strunk, W. Jr. and White, E.B., “The Elements of Style”, Allyn and Bacon, 4th Edn.	2003

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-521 Course Title: **Advanced Analytical Methods**
2. Contact Hours: **L: 3** **T: 1** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 4** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Basic knowledge in analytical chemistry
9. Objective: To impart knowledge on various instrumental analytical methods.
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Chromatographic separation techniques:** van Deemter equation, processes leading to non-ideal chromatography; theory, instrumentation and applications of gas chromatography, high performance liquid chromatography; types of columns, impregnated, bonded and crosslinked stationary phases, Kovat's index; ion chromatography; size exclusion chromatography; affinity chromatography; electrophoresis.	**8**
2.	**Mass spectrometry and hyphenated systems:** Types of ion sources, mass analysers and detectors, resolution, nitrogen rule, ring rule, interpretation of data and applications, hyphenated techniques- GC-MS, LC-MS, MS-MS, examples.	**5**
3.	**Electroanalytical techniques:** Principle, instrumentation and applications of AC polarography, rapid scan, pulse, square wave, anodic stripping and cyclic voltammetric methods.	**4**
4.	**Atomic spectroscopy:** Optical atomic spectra, atomic linewidth and line broadening, sample atomization techniques, hydride generation, cold vapour technique, instrumentation of atomic absorption spectroscopy, interferences in atomic absorption spectroscopy and their correction methods, inductively coupled plasma optical emission spectroscopy and inductively coupled plasma mass spectrometry and applications.	**8**
5.	**Radiochemical methods:** Generation of radioisotopes as radiotracers, radiolabelling, radioactivity measurement- GM-counter, NaI (Tl) scintillation detector, semiconductor detectors, applications of radioisotopes – Mossbauer spectroscopy; positron annihilation spectroscopy; activation analysis.	**6**
6.	**Thermal methods of analysis:** Instrumentation on thermogravimetric analysis (TGA); differential thermal analysis (DTA); differential scanning calorimetry (DSC); thermogravimetry coupled with mass spectrometer (TG-MS) and infrared spectrophotometer (TG-FT-IR).	**3**
7.	**Automated methods of analysis:** Importance of automation in chemical analysis, types of automated system, segmented and continuous flow, flow injection analysis – principle, instrumentation, applications; stopped flow method, sequential injection analysis, discrete analyzer, automated organic elemental analyser. Microfluidic devices in analytical chemistry, lithographic techniques for fabrication of microfluidic devices.	**8**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
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.	Christian, G.D., Dasgupta P.K., Schug K.A., "Analytical Chemistry", 7th Ed., John Wiley & Sons Inc.	**2013**
4.	Bond, A.M., "Modern Polarographic Methods in Analytical Chemistry". 1st Ed., CRC Press.	**1980**
5.	Sood, D.D., Reddy A.V.R. and Ramamoorthy N., "Fundamentals of Radiochemistry", IANCAS Publication, BARC, Mumbai	**2004**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-523 Course Title: **Organic Chemistry V**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Autumn** 7.Subject Area**: PCC**
8. Pre-requisite**:** Basic concepts in chemistry of hydrocarbons
9. Objective: To impart knowledge in synthetic organic chemistry
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Functional Group Transformations :** Introduction of functional groups (alcohols, halides, nitriles, amines, azides) by substitution at saturated carbon, cleavage of ethers, esters and amides, interconversion of nitriles and carboxylic acid derivatives (esters, acids, acid chlorides, amines), protecting groups – acetals, ethers, silyl ethers and esters, protection of diols, amines, carbonyls and carboxylic acids.	**10**
2.	**Main group metals mediated synthesis :** Addition reactions of electrophilic sulfur and selenium reagents, iodolactonization, sulfenylcyclization, selenenylcyclization, α-sulfenylation and α-selenylation to carbonyl compounds, hydroboration of alkenes and alkynes, reactions of organoboranes, enantioselective hydroboration; hydroalumination, carboalumination.	**8**
3.	**Reductions :** Reduction of alkenes, alkynes, hydrogenation using heterogeneous and homogeneous catalysts, enantioselective hydrogenation, hydrogen transfer reagents, hydrogenation of carbonyls, hydrogenolysis, hydrogen donor reagents - $NaBH_4$, $LiAlH_4$ and modified reagents, silicon hydrides, tin hydrides; reduction of imines, imides and amides, chemoselectivity and stereoselectivity of reductions, enantioselective reduction of carbonyl compounds, Meerwein-Ponndorf-Verley reduction, dissolving metal reductions, McMurry coupling, Clemmensen reduction, Wolff-Kishner reaction, Shapiro reaction.	**12**
4.	**Oxidations :** Oxidation of alcohols- Jones reagent, Swern oxidation, Dess-Martin reagent; dihydroxylation of alkenes, metal catalyzed epoxidation of alkenes, Sharpless asymmetric epoxidation, epoxidation by peroxy reagents, dioxirane derivatives, nucleophilic and reductive ring opening of epoxides, rearrangements of epoxides, oxidation of allyl compounds, selenium derivatives as oxidants, oxidative cleavage of alkenes, ozonolysis, oxidation of aldehydes and ketones, Baeyer-Villiger oxidation, oxidation of enolates, glycols, carboxylic acids and non-functionalized carbons.	**12**
	Total	**42**

11. Suggested Books:

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Larock, R.C. “Comprehensive Organic Transformations”, John Wiley & Sons	**2018**
2.	Carey, F.A. and Sundberg, R.J. “Advanced Organic Chemistry. Part B: Reaction and Synthesis”, Springer.	**2008**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-525 Course Title: **Advanced Molecular Spectroscopy**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Quantum chemistry, group theory and basic concepts in spectroscopy
9. Objective: To impart knowledge on some of the widely used spectroscopic methods for understanding molecules and compounds.

10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Optical rotatory dispersion and circular dichroism**: Optical activity, Basic principles of optical rotatory dispersion and circular dichroism, Cotton effect, Selection rules – magnetic transition moment, rotational strength, absolute configuration, spectropolarimeter, applications	**4**
2.	**Nonlinear spectroscopy:** History of nonlinear optics, theoretical foundations, second harmonic generation, phase matching, symmetry considerations, optical rectification, Pockels effect, sum frequency generation, difference frequency generation and optical parametric amplification, third order processes.	**6**
3.	**Nuclear magnetic resonance:** Nuclear magnetism, nuclear spin states in a magnetic field and the resonance phenomenon, relaxation processes and their importance. Bloch equation, Larmor frequency, shielding constant and chemical shifts. Factors affecting chemical shifts – local diamagnetic shielding, magnetic anisotropy of chemical bond, hydrogen bonding effect; spin-spin coupling and quantum chemical description of spin systems-spectra AX_2 and AX_3 spin systems, spectra of AMX and AMX_n spin systems. Chemical exchange process, spin decoupling, dynamic NMR and line shapes. double resonance experiments and nuclear overhauser effect, chemical shift reagents, NMR spectra of ^{13}C, ^{19}F and ^{31}P systems; solid state NMR, magic angle, 2D NMR.	**14**
4.	**Electron spin resonance:** g-factor, interaction of magnetic dipole with microwave radiation, hyperfine splitting from proton and from nuclei with spin greater than ½, hyperfine interaction, anisotropic system; triplet state – spin transition, effect of dipolar field, zero field splitting, spectrum of naphthalene triplet, spectral interpretation - g-value determination, complexes of transition metals ions, double resonance techniques	**8**
5.	**X-ray Absorption spectroscopy**: X-ray emission spectrum, X-ray absorption spectrum, XANES and EXAFS – theory and applications in inorganic materials.	**4**
6.	**Mossbauer Spectroscopy**: Principles, experimental details – line width and recoil energy; Mossbauer spectral parameters – isomer shift, electric quadrupole interaction, magnetic splitting; applications with ^{57}Fe and ^{119}Sn systems.	**6**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Sathyanarayana, D.N. "Handbook of Molecular Spectroscopy from Radiowaves to Gamma rays". IK International Publishing House Pvt. Ltd., New Delhi	**2015**
2.	Banwell, C.N. and McCash, E.L.M. "Fundamentals of Molecular Spectroscopy", 4th Ed. McGraw-Hill N. Y	**1999**
3.	Graybeal, J.D. "Molecular Spectroscopy", 1st Rev. Edn, McGraw-Hill	**2014**
4.	Gunther, H. "NMR spectroscopy", 2nd Edition, Wiley-India	**2010**
5.	Poole, C.P., "Electron Spin Resonance, A Comprehensive Treatise on Experimental Techniques", 2nd Edition, Dover Publications Inc, NY	**1996**
6.	Boyd R.W., "Nonlinear Optics", 3rd Edn, Academic Press	**2008**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-531 Course Title: **Laboratory III**
2. Contact Hours: **L: 0** **T: 0** **P: 12**
3. Examination Duration (Hrs.): **Theory 0** **Practical 6**
4. Relative Weightage**: CWS 0** **PRS 50** **MTE 0** **ETE 0** **PRE 50**
5. Credits**: 6** 6. Semester**: Autumn** 7.Subject Area**: PCC**
8. Pre-requisite**:** Knowledge in different areas of chemistry
9. Objective: To provide knowledge in laboratory based experiments
10. Details of the Course:

Physical Chemistry

1. To study the kinetics of H^+ catalyzed hydrolysis of an ester.
2. To study the kinetics of saponification of an ester.
3. To study the kinetics of Fe^{3+} catalyzed decomposition of hydrogen peroxide.
4. Determine the composition of KCl-KBr mixtures by potentiometric titration against silver nitrate solution.
5. To study the quenching of fluorescence of organic dye(s).
6. To determine the molecular weight of a volatile substance using Victor Meyer method.
7. To determine the cell potentials for different electrochemical cells and also to measure different thermodynamic parameters.

Inorganic Chemistry

1. Synthesis of nickel complexes e.g., $[Ni(H_2O)_6]^{2+}$, $[Ni(NH_3)_6)^{2+}$ and $[Ni(en)_3]^{2+}$ for
   (a) Comparison of the electronic spectra;
   (b) Qualitative verification of the spectrochemical series, and
   (c) Quantitative estimation of nickel by spectrophotometry
2. Synthesis and spectrophotometric study of bis(salicylaldimine)copper(II) and cis-bis(glycinato)copper(II),
3. Record spectra of Cu^{2+} in water, NH_3, ethylene diamine and glycine, and arrange the ligands in increasing order of field strength.
4. Quantitative estimation of copper by spectrophotometry.
5. (i) Study of the complex formation between Fe(III) and thiocyanate/salicylic acid/sulphosalicylic acid or between Ni(II) and *o*-phenanthroline;
   (ii) spectrophotometric determination for formation constant of the metal complex (Job's method and molar ratio method).
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 characterization by FT-IR, UV-vis and ^1H NMR spectroscopy.
7. Synthesis of potassium tris(oxalato)aluminate, potassium tris(oxalato)chromate and potassium tris(oxalato)ferrate, and their characterization by metal determination, various spectroscopic (I.R. and UV-vis) methods, magnetic moment determination, and photochemical behavior of iron complex.
8. Synthesis and characterization of $[Co(en)_3]Cl_3$. Separation of its optical isomers and determination of their optical rotation by using polarimeter.

Organic Chemistry

1. Fisher indole synthesis (2 turns)
2. Preparation of trans-9-(2-phenylethenyl)anthracene from anthracene (formylation and Wittig reaction). (2 turns)
3. Synthesis of *N*-benzylbarbituric acid from diethylmalonate (2 turns)
4. Luminol synthesis and chemiluminescence (3 turns)
5. Synthesis of hexaphenylbenzene from diphenylacetone and *E*-stilbene or benzil via cyclopentadienone and diphenylacetylene. (5 turns)

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-522 Course Title: **Materials Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Spring** 7. Subject Area**: PCC**
8. Pre-requisite**:** Knowledge in solid state chemistry
9. Objective: To provide knowledge on materials chemistry, synthesis, characterization and properties of materials

10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Introduction:** Historical perspective, classifications, approaches to produce new materials, role of chemistry in material science and applications, role of structure, composition and bonding on the properties of materials.	**4**
2.	**Synthesis of materials:** Conventional methods - colloidal synthesis, precipitation and co-precipitation, sol-gel synthesis, ceramic method, combustion method, arc melting, mechanical attrition. Non-conventional methods: hydrothermal and solvothermal, electrochemical reduction, sonochemistry, microwave assisted synthesis, arc discharge, biomineralization and biomimetic synthesis. Soft-chemistry methods: ion-exchange, intercalation and exfoliation. Thin film growth - dip coating, spin-coating, chemical vapour transport, metal organic chemical vapour deposition, sputtering, pulsed laser deposition,atomic layer deposition.	**14**
3.	**Materials based on composition:** Metals and alloys, semiconductors, ceramics, zeolites and glasses, organic soft materials/molecular materials, liquid crystals, polymers and composites, carbon based materials and biomaterials.	**5**
4.	**Materials based on morphology and microstructure**: Powders, thin films, monoliths, amorphous materials; nanomaterials –nanocrystals, porous materials, photonic crystals.	**5**
5.	**Application of materials:** structural materials, optical materials, superconducting materials, thermoelectric materials, magnetic materials, dielectrics, multiferroics, energy materials (supercapacitors, batteries, fuel cells, solar cell, hydrogen storage and nuclear materials), materials for healthcare, materials for environmental remediation (control of greenhouse gas emission and water treatment).	**14**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Allcock, H.R., "Introduction to Material Chemistry" John Wiley & Sons, Inc.	2008
2.	Fahlman, B.D., "Material Chemistry" Springer	2011
3.	Klabunde, K.J., and Richards, R.M. "Nanoscale Materials in Chemistry" K. J. Klabunde, R. M. Richards, 2nd Edn., John Wiley & Sons, Inc.	2009
4.	Callister, Jr. W. D. and Rethwisch, D. G. "Material Science and Engineering: An Introduction" 8th Edn., John Wiley & Sons, Inc.	2009
5.	Delhaes, P. "Carbon-based Solids and Materials". John Wiley & Sons,Inc.	2011
6.	West, A.R., "Solid State Chemistry and its Applications" Wiley India	2013

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-524 Course Title: **Frontier Inorganic Chemistry**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Spring** 7. Subject Area**: PCC**
8. Pre-requisite**:** Knowledge in coordination chemistry and organometallics
9. Objective: To impart advanced knowledge in Inorganic Chemistry
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Advanced Organometallic Chemistry:** Metallocene catalysis for olefin polymerization, catalytic cycle for hydrosilation and hydrocyanation, Davies-Green-Mingos rule for organometallic clusters, Kuba's dihydrogen complex, synthesis of CCC-chelates using Os complexes, organometallic dendrimers with Fe and Pt, third generation Grubb's catalyst for ring opening polymerization, decarbonylation of acid chlorides, reaction of metal acyl enolates with electrophile, C-H activation and use of weakly coordinating anions, alkane metathesis, heterogeneous catalysis for organic transformations using organometallic frameworks of Zn-Pd and Co.	**8**
2.	**Reaction mechanisms:** Substitution reactions in octahedral complexes– exchange reactions, acid- and base-hydrolysis, anation, solvolytic and catalyzed reactions. Substitution reactions in square-planar complexes–effect of non-participation of ligands on reactivity, *cis* and *trans* effects, outer- and inner-sphere mechanisms, factors affecting electron transfer reaction rates, theories of electron transfer reactions, solvated electron, photochemically excited states and excited state processes for transition metal complexes, photochemical reactions of coordination compounds.	**14**
3.	**Bioinorganic chemistry:** Metalloproteins and enzymes– role of metal ions in the active sites, structural and functional models 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, catalases, peroxidases,pseudocatalase, hydrolases, oxygen carriers- haemoglobin, myoglobin; non-haem proteins- hemerythrin, hemocyanin, Fe-ribonucleotidereductase, cytochrome c oxidases, cytochrome P-450s, Ni-urease, hydrogenase, nitrogen fixation, blue copper proteins, tyrosinase, galactose oxidase, superoxide dismutases, carbonicanhydrase, carboxypeptidase, alcohol dehydrogenase. Roles of transition metals (Ti, V, Fe, Co, Tc, Hg, Pt, Au and Ru) in biology and medicine.	**20**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Crabtree, R. H. "The Organometallic Chemistry of Transition Metals" 6th ed. John Wiley & Sons.	**2014**
2.	Huheey, J.E., Keiter, E.; Keiter, R. and Medhi, O.K., "Inorganic Chemistry: Principles of Structure and Reactivity", 4th Ed., Pearson Education Asia.	**2006**
3.	Gibbs, W., "Concepts and Applied Principles of Bioinorganic Chemistry", Vol. III Callisto Reference.	**2015**
4.	Gupta, B. D., Elias, A. J. "Basic Organometallic Chemistry" 2nd Edition, University Press (India) Pvt Ltd	**2013**
5.	Lippard, S.J. and Berg, J., "Principles of Bioinorganic Chemistry", University Science Books, U.S.A.	**1994**
6.	Bertini, I., Gray, H.B., Lippard, S.J. and Valentine, J.S., "Bioinorganic Chemistry", University Science Books, U.S.A.	**1994**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-526 Course Title: **Organic Chemistry VI**
2. Contact Hours: **L: 3** **T: 0** **P: 0**
3. Examination Duration (Hrs.): **Theory 3** **Practical 0**
4. Relative Weightage**: CWS 20-35 PRS 0 MTE 20-30 ETE 40-50 PRE 0**
5. Credits**: 3** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Knowledge of functional groups in organic chemistry and their reactivity
9. Objective: To develop concepts in structure elucidation in Organic Chemistry
10. Details of the Course:

Sl. No.	Contents	Contact Hours
1.	**Infrared Spectroscopy**: Factors influencing vibrational frequencies, interpretation of IR spectra, characteristic group absorptions of hydrocarbons, aromatic systems, alcohols, phenols, ethers, carbonyl compounds, amines, nitriles and related compounds, nitro, sulfur and phosphorous compounds, alkyl halides and aryl halides	**4**
2.	**UV-vis Spectroscopy**: Solvent effect, chromophores, auxochromes, effect of conjugation; empirical rules to predict λ_{max} for dienes, enones and α,β-unsaturated aldehydes and acids; aromatic compounds, polynuclear aromatic hydrocarbon and heterocyclic compounds, electronic transition for charge transfer complexes, keto-enol tautomerism.	**5**
3.	**Mass Spectrometry**: Determination of molecular formula, isotope effects, nitrogen rule, McLafferty rearrangement, metastable ions, fragmentation patterns of acyclic and cyclic hydrocarbons, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, nitrogen and sulfur compounds, alkyl halides.	**5**
4.	**NMR Spectroscopy**: Fundamentals of NMR sensitivity and resolution, chemical shift, chemical and magnetic equivalence, shielding, magnetic anisotropy, origin of spin-spin splitting, (n+1) rule, chemical shifts of common NMR solvents, NMR spectra at low and high field strengths, deuterium exchange experiments, coupling constant, types of coupling – vicinal, geminal, long-range; 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, ^{1}H NMR spectra of compounds of various functional groups, nuclear Overhauser effect.	**14**
5.	**^{13}C and heteronuclear NMR Spectroscopy**: Introduction to ^{13}C NMR, chemical shifts in ^{13}C NMR, proton-coupled and decoupled ^{13}C NMR, chemical shifts of common NMR solvents, DEPT spectroscopy. NMR spectroscopy of other common NMR-active nuclei such as ^{15}N, ^{19}F, ^{29}Si, and ^{31}P.	**5**
6.	**Two-dimensional NMR Spectroscopy**: 2D NMR techniques – homo- and hetero-nuclear correlation (COSY, HETCOR, TOCSY, HSQC, HMBC), NOESY, ROESY and INADEQUATE.	**5**
7.	**Structure elucidation of complex molecules**: Solving structures utilizing IR, UV, MS, NMR data.	**4**
	Total	**42**

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprints
1.	Silverstein, R.M., Webster, F.X., Kiemle, D.J. and Bryce, D.L. "Spectrometric Identification of Organic Compounds", 8th Edn., Wiley.	2014
2.	Pavia, D.L. Lampman, G.M., Kriz, G.S. and Vyvyan, J.A. "Introduction to Spectroscopy", 5th Edn., Cengage Learning.	2015
3.	Uauglitz, G and Vo-Dinh, T. (Eds), "Handbook of Spectroscopy", Wiley.	2003
4.	Pretch, E., Bühlmann, P and Badertscher, M. "Strucutre Determination of Organic Compounds", Springer.	2009
5.	Field, L.D., Sternhell, S., Kalman, J. R. "Organic Structures from Spectra", 4thEdn, Wiley.	2008
6.	Simpson, J.H. "Organic Structure Determination using 2-D NMR Spectroscopy", Academic Press.	2008

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: CYN-532 Course Title: **Laboratory IV**
2. Contact Hours: **L: 0** **T: 0** **P: 12**
3. Examination Duration (Hrs.): **Theory 0** **Practical 6**
4. Relative Weightage**: CWS 0** **PRS 50** **MTE 0** **ETE 0** **PRE 50**
5. Credits**: 6** 6. Semester**: Autumn** 7. Subject Area**: PCC**
8. Pre-requisite**:** Basic knowledge of synthesis, characterization and analysis of compounds
9. Objective: To provide advanced level laboratory based experiments
10. Details of the Course:

Name of the experiments:

1. Separation of binary mixture of organic compounds using column chromatography.
2. Simultaneous spectrophotometric determination of concentration of $KMnO_4$ and $K_2Cr_2O_7$ in a given mixture.
3. Determination of Na, K in a soil sample by flame photometry.
4. Determination of metal in alloy samples by AAS.
5. Radiation measurement by NaI(Tl) and GM counter.
6. Determination of metal ions by polarography and voltammetry methods.
7. Extraction of Fe^{3+} using 8-hydroxyquinoline.
8. Catalytic oxidation of organic substrates and analysis by GC.
9. Structure elucidation of organic molecules using ^{1}H and ^{13}C NMR spectra.
10. Synthesis, characterization and applications of ZnO or CdS or CdSe nanoparticles
11. Literature search in organic chemistry using e-sources
12. Michael addition followed by Robinson annulation: Reaction of methylvinyl ketone with aldehyde or ketone.
13. Preparation of anthracene from phthalic anhydride.
14. Esterification and nitration of *p*-hydroxybenzoic acid.
15. Synthesis of 4-cyano-2-aminophenol from 4-hydroxybenzaldehyde.
16. 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.
17. Magnetic measurement: Synthesis of iron/chromium complexes and their characterization by IR, UV-Vis spectrometry, Magnetic measurements and photochemical studies.

LIST OF PECs

For Autumn Semester:

1. Separation Techniques and Microanalysis (CYN-605)
2. Electroanalytical Chemistry (CYN-607)
3. Frontiers in Bioinorganic Chemistry (CYN-613)
4. Crystal and Molecular Structure (CYN-615)
5. Supramolecular Chemistry (CYN-617)
6. Organic Semiconductors (CYN-623)
7. Proteins and Polypeptides (CYN-625)
8. Advanced Surface and Colloidal Chemistry (CYN-627)
9. Advanced Physical Chemistry (CYN-629)
10. Nanoscale Materials: Properties and Applications (CYN-633)
11. Advanced Magnetic Resonance Spectroscopy (CYN-635)
12. Analysis of Industrial Polymers (CYN-751)

For Spring Semester:

1. Nuclear and Radiochemistry (CYN-512)
2. Heterocyclic Chemistry (CYN-514)
3. Total Synthesis (CYN-606)
4. Chemical Biology (CYN-608)
5. Molecular Modeling and Simulations (CYN-610)
6. Carbon Nanomaterials and their Applications (CYN-612)
7. Pharmaceutical Organic Synthesis (CYN-722)
8. Environmental Chemistry (CYN-732)
9. Analysis of Materials (CYN-742)
10. Analysis of Food and Drugs (CYN-752)
11. Chemistry of Industrial Processes (CYN-782)

Note: all the above PECs are Senate Approved 3-credit courses.