

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-702** Course Title: **Chemistry of Materials**

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

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

4 Relative Weightage: **CWS 20-30 PRS 0 MTE 20-30 ETE 40-60**

5. Credits: **3** 6. Semester: **Autumn/Spring** 7. Subject Area: **Pre-Ph.D.**

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

9. Objective: To provide knowledge on materials chemistry, synthesis, characterization, properties and applications of materials

10. Details of Course:

S. No.	Contents	Contact Hours
1.	Introduction to chemistry of materials. Historical perspective, classification schemes, approaches to produce new materials, role of chemistry in material science and applications, role of bonding, structure and composition, powders, thin films, monoliths, porous materials, amorphous materials, nanomaterials.	4
2.	Types of materials. Metals and alloys; Semiconductors; Ceramics-conventional and modern ceramics; Polymers and composites-types, biopolymers and inorganic polymers; Metamaterials; Carbon-based materials-carbon nanotubes, fullerenes, graphene and other carbon nanomaterials.	10
3.	Synthesis of materials. Conventional synthetic methods: colloidal synthesis, precipitation and co-precipitation, hot injection, sol-gel synthesis, ceramic method, mechanical attrition. Non-conventional synthetic methods: hydrothermal and solvothermal, electrochemical reduction, sonochemistry, microwave-assisted synthesis, and biomineralization; Soft-chemistry methods: ion-exchange, intercalation and exfoliation; Thin film growth: dip coating, spin-coating, chemical vapor deposition, chemical vapor transport, atomic layer deposition and pulsed laser deposition method	14
4.	Properties and applications. Structural, optical, superconducting, thermoelectric and magnetic materials; dielectrics; energy materials - supercapacitors, batteries, fuel cells, solar cells, hydrogen storage and nuclear materials; materials for healthcare; materials for environmental remediation - control of greenhouse gas emission, sequestration and utilization, water treatment.	14
	Total	42

11. Suggested Books:

Sl. No.	Authors/ Title/ Publisher	Year of Publication

1.	"Introduction to Material Chemistry" Allcock H. R., <i>John Wiley & Sons, Inc.</i>	2008
2.	"Material Chemistry" Fahlman B. D., <i>Springer</i>	2011
3.	"Nanoscale Materials in Chemistry" Klabunde K. J., Richards R. M., 2 nd edn., <i>John Wiley & Sons, Inc.</i>	2009
4.	"Material Science and Engineering: An Introduction" Callister Jr W. D., Rethwisch D. G., 8 th edn., <i>John Wiley & Sons, Inc.</i>	2009
5.	"Carbon Nanomaterials" Mathur R. B., Singh B. P., Pande S., <i>Taylor & Francis</i>	2017
6.	"Solid State Chemistry and its Applications" , West A. R., Reprint, <i>Wiley India</i>	2013
7.	"Introduction to Ceramics" , Kingery W. D., Bowen H. K., Uhlmann D. R., <i>Wiley-Interscience</i>	1976
8.	"Introduction to Polymer Science and Chemistry" , Chanda M., <i>Taylor and Francis</i>	2006

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-703** Course Title: **Advanced Materials Characterization Techniques**

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

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

4 Relative Weightage: **CWS 20-30 MTE 20-30 ETE 40-60**

5. Credits: **4** 6. Semester: **Autumn/Spring** 7. Subject Area: **Pre-Ph.D.**

8. Pre-requisite: **Basic knowledge in chemistry and physics**

9. Objective: To provide knowledge on characterization of materials

10. Details of Course:

S. No.	Contents	Contact Hours
1.	X-ray diffraction. Concept of lattice, crystalline state, types of crystal system and structures, X-ray sources, filters and monochromators, detectors, principle of X-ray diffraction, amplitude and phase of diffraction, structure factors, systematic absences, experimentation – powder method, interpretation of diffraction data – indexing and lattice parameters, lattice parameter refinement and pattern simulation, Rietveld refinement using X-ray data.	10
2.	Microscopic techniques. Principle of electron-matter interaction, transmission electron microscope (TEM) -instrumentation, electron sources – field emission, condenser lenses, objective lenses, sample stage, image creation- bright field and dark field images, specimen preparation, electron diffraction pattern and indexing, high resolution TEM; scanning electron microscope - instrumentation, secondary and back scattered electron images, energy dispersive X-ray analysis and elemental mapping; atomic force microscopy - concepts and instrumentation	10
3	Texture analysis. N ₂ sorption, adsorption isotherms-BET and Langmuir, method for estimation of specific surface area, pore size distribution, pore volume analysis of porous materials.	4
4.	X-ray photoelectron spectroscopy. Electronic structure of atoms and ions, stationary state notation, photoelectric effect and work function; instrumentation-vacuum level, X-ray sources, electron sources, ion sources, energy analyser, detector, imaging; data collection and quantification - analysis procedures, photoelectron intensities, depth profiling, spectral interpretation - binding energy and chemical shifts; case studies.	7
5.	Thermal and magnetic measurements. Thermogravimetric analysis, differential thermal analysis, differential scanning calorimetry; magnetic susceptibility, hysteresis (M-H), field-cooled and zero field-cooled measurements, magnetization, VSM and SQUID magnetometry; AC susceptibility, case studies.	6
6.	Optical and Raman spectroscopy. Diffuse reflectance spectroscopy, ATR, photoluminescence, Raman spectroscopy-principle, instrumentation and application in carbonaceous materials, metal oxides and chalcogenides.	5
	Total	42

11. Suggested Books:

Sl. No.	Authors/ Title/ Publisher	Year of Publication
1.	"Principles of Instrumental Analysis " Skoog D.A., Holler F.J., and Crouch S.R., <i>6th Ed., Cengage</i>	2014
2.	"Solid State Chemistry and its Applications" West A.R., <i>John Wiley & Sons</i>	2002
3.	"Transmission Electron Microscopy: A textbook for Materials Science" Williams D.B. and Carter C.B., 2nd Edition, Springer	2003
4.	"Scanning Electron Microscopy and X-Ray Microanalysis" Goldstein, J., Newbury, D.E., Joy, D.C., Lyman, C.E., Echlin, P., Lifshin, E., Sawyer, L and Michael J.R., 3rd Edition, Springer	2003
5.	"X-ray Photoelectron Spectroscopy: An Introduction to Principles and Practices" Van der Heide, P., <i>John Wiley & Sons</i>	2012
6.	"Surface Area and Porosity Determinations by Physisorption" Condon, J., <i>Elsevier Science</i>	2006
7.	"Magnetic Materials: Fundamentals and Device Applications" Nicola, S., <i>Cambridge University Press</i>	2003

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-901** Course Title: **Research Methodology in Chemical Sciences**

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

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

4. Relative Weightage: **CWS 20-30 PRS 0 MTE 20-30 ETE 40-60 PRE 0**

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

8. Pre-requisite: **NIL**

9. Objective: To introduce research ethics and methodologies for scientific research and writing in chemistry

10. Details of the Course:

Sl. No.	Contents	Contact Hours
1	Overview of chemistry research: Objectives of research, importance of research methodology in chemistry research, general principles of research design, types and methods of research, identification of research-problem, and statement of research problem.	3
2	Chemical literature survey: Sources of information, need for reviewing literature, primary-secondary-tertiary sources, journals, journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text books, current contents; TOC alerts, Search engines (Google scholar, SciFinder, Beilstein, Web of Science, Scopus), publication ranking analytics, author identification – ORCID and Publons ID.	4
3	Chemistry data presentation tools: Use of drawing tools such as Excel, SigmaPlot, Origin, Matlab, ChemDraw and open source software; plotting of various spectra, images and diagrams.	5
4	Methods of chemistry research: Inculcation of scientific temper, avoidance of prejudices and lax judgements, impulses of a strong will to do research, persistent hard work and concentration, developing high-minded independence of judgement and thirst for scientific originality, planning of research, formulation of selected problems, hypothesis formation, design and execution of experiments, collection and interpretation of experimental data, observation, arriving at conclusions; Maintaining logbooks, documentation of experiments and data in laboratory notebook, importance of safety and security of data.	5
5	Documentation and presentation of research output: Reporting the results of research - style and format, title, abstract and the text, abbreviations, tables, figures, legends, elucidations, quotations and footnotes, references; Guidelines of presentation of data, typesetting, templates, formulas and equations, reference formats, supplementary data; Writing style for communications, perspectives, review articles, accounts monographs, dissertations and theses; drafting, refinement, common errors, editing services, proof reading; Presentation modes – board, poster, power-point, audio-visual.	6

6	Ethics in research: Authorship, citation and acknowledgement, reproducibility of results, plagiarism, similarity check, duplicate and redundant publications, predatory publishing, open access licenses, embargo period, repositories, conflicts of interest, bio-ethics, social networks for promotion, intellectual property rights.	3
7	Chemical and laboratory safety: Safety rules of laboratory, MSDS, disposal of chemical wastes, use of fire extinguisher, first aid and antidotes.	2

11. Suggested Books

Sl. No.	Authors/ Title/ Publisher	Year of Publication/ Reprint
1.	Hoffman, A., "Scientific writing and communication", 2 nd Ed., Oxford University Press.	2014
2.	Katz, M. J., "From Research to Manuscripts: A Guide to Scientific Research", 2 nd Ed, Springer.	2009
3.	Ebel, H. F., Bliefert, C., and Russey, W. E., "The art of scientific writing", 2 nd Ed, Wiley-VCH.	2004
4.	Kothari, C. R., "Research Methodology Methods and Techniques", 2 nd Ed, Vishwa Prakashan.	2006
5	"Chemical safety matters–IUPAC–IPCS", Cambridge University Press.	1992

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-902** Course Title: **Advanced Inorganic Chemistry**
2. Contact Hours: **L: 03 T: 0 P: 0**
3. Examination Duration (Hrs.): **Theory 3 Practical 0**
4. Relative Weightage: **CWS 20-30 PRS 0 MTE 20-30 ETE 40-60 PRE 0**
5. Credits: **3** 6. Semester: **Autumn/Spring** 7. Subject Area: **PEC**
8. Pre-requisite: **NIL**
9. Objective: To familiarise the students with recent topics required for inorganic chemistry research
10. Details of Course:

S. No.	Contents	Contact Hours
1	Applications of Group Theory in Inorganic Chemistry: Spectroscopic term symbols for free ions, metal complexes in octahedral, tetrahedral, square planar, square pyramidal complexes; use of irreducible representations for translations, rotations and vibrations in these molecules and their theoretical interpretation for infra-red and Raman transitions.	14
2	Current trends in Organometallic Chemistry: Organometallic approach to water splitting, role of osmium, ruthenium, titanium, manganese complexes in water splitting, homolytic activation of water with nickel, closed circle water splitting model, E-H bond activation of ammonia and water by phosphorous compounds, oxygen atom transfer reactions, role of pincer ligands, multimetallic catalysis based on heterometallic complexes.	14
3	Current trends in Bioinorganic Chemistry: Biological and synthetic oxygen carrier, platinum anticancer drugs and interaction of cisplatin with glutathione in cancer cell, types of superoxide dismutases – their active site structure and reaction mechanism, dioxygen activation by iron and copper enzymes, biomineralization, scorpionate ligands and hybrid materials for metalloenzyme models.	14

11. Suggested books:

S. No.	Authors/Title/Publishers	Year of Publication/ Reprint
1	Cotton, F. A. "Chemical Application of Group Theory" Wiley Student Edition, 3 rd ed.	2008

2	Crabtree, R. H., "Organometallics and Catalysis: An Introduction", Wiley, 6 th ed.	2014
3	Hartwig, J. F., "Organotransition Metal Chemistry: From Bonding to Catalysis", University Science Books.	2010
4	Research papers on the above mentioned topics	2019

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-903** Course Title: **Advanced Organic Chemistry**
2. Contact Hours: **L: 03 T: 0 P: 0**
3. Examination Duration (Hrs.): **Theory 3 Practical 0**
4. Relative Weightage: **CWS 20-30 PRS 0 MTE 20-30 ETE 40-60 PRE 0**
5. Credits: **3** 6. Semester: **Autumn/Spring** 7. Subject Area: **PEC**
8. Pre-requisite: **NIL**
9. Objective: To familiarise the students with recent topics required for organic chemistry research
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	Art in organic synthesis: General considerations (realistic mechanisms, HSAB concept, Curtin-Hammett principles, homogeneous or heterogeneous systems, thermodynamic allowance, linear vs convergent methods), oxidation level of carbon centers in functional groups, isohypsic and non-isohypsic reactions, synthetic equivalency of functional groups, design of chemoselective, regioselective and stereoselective reactions, renewable feedstocks as synthons, umpolung in synthesis, synthesis of cyclic molecules, radical reactions for cyclisations (Corey's γ -lactone synthesis)	8
2.	Side reactions in Organic Synthesis: Stability of organic compounds, stability towards oxygen (H-abstraction, SET mechanism), strained bonds, incompatible functional groups, detonating compounds, nature of electrophiles in nucleophilic substitution, effects of heteroatoms in electrophiles (nitrogen, halogen, silicon, boron), allylic and propargylic electrophiles, acylation reaction with problematic amines and alcohols (sterically and electronically deactivated amines, aminoacids, base labile alcohols), β -hydride elimination, protodemetalation, dimerization as major side reactions in transition metal catalyzed organic synthesis	6
3.	Green chemistry in organic synthesis: Principles of green chemistry, atom economy and scope, preparation of green matrix, alternatives to common organic synthetic methods, microwave assisted organic synthesis (equipment, activation benefit, limitations, microwave effects in synthesis, some exemplary synthesis under microwave irradiation), visible light photochemistry (fundamentals of photocatalysis, metal complexes and organic dyes as photocatalysts, visible light photocatalysis in C-H activation reactions, atom transfer radical addition reaction, difunctionalization of alkenes and alkynes, α -amino functionalization reactions), organic synthesis in water (basic requirements, in-water and on-water synthesis, formation of trans phase, exemplary methods), mechanochemistry (ball mills in organic synthesis, use of stress in cleaving bonds, exemplary methods), organocatalysis (Aldol reaction, acyl transfer reactions, Setzer reaction, Baker's yeast, N-heterocyclic carbenes) Ionic liquids (introduction and application in organic synthesis).	14
4.	Modern methods of heteroaromatic synthesis: Systematic nomenclature of heterocyclic compounds (Hantzsch Widman, replacement and fusion methods), synthesis of heterocyclic compounds based on transition metal catalyzed chemistry using Cu, Pd, Co and Ni (transition-metal-catalysed carbene coupling reactions, tandem catalytic reactions, carbonylation of acyclic precursors, cycloisomerizations of allenes with amine, amide, or sulfonamide nucleophiles, incorporation of chemo-, regio-, and stereocontrol in heterocyclic synthesis), synthesis and reactivity of hypervalent iodine compounds, applications of hypervalent iodine(III) reagents in the constructions of heterocyclic compounds through oxidative coupling reactions, multicomponent reactions, use of	14

	multicomponent reactions in heterocyclic synthesis, Biginelli condensation, Kabachnik–Fields reaction, van Leusen method, Ugi reaction, Passerini Reaction and their postcondensation modifications, Knoevenagel-induced domino reactions, synthesis of heterocycles in nature, applications of heterocycles in pharmaceuticals, materials and agrochemicals	
	Total	42

11. Suggested Books

S. No.	Name of Authors /Books/Publishers	Year of Publication/ Reprint
1.	Smit, W. A., Bochkov, A. F., Caple, R., "Organic Synthesis, The Science behind the Art", The Royal Society of Chemistry, London.	1998
2.	Dörwald, F. Z., "Side Reactions in Organic Synthesis, A Guide to Successful Synthesis Design", WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim	2005
3.	Lancaster, M., "Green Chemistry, an Introductory Text", The Royal Society of Chemistry, London.	2002
4.	Kotschy, A., Timári, G., "Heterocycles from Transition Metal Catalysis, Formation and Functionalization", Springer, The Netherlands.	2005
5	Orru, R. V. A., Ruijter, E. (Ed), "Synthesis of Heterocycles via Multicomponent Reactions I, Springer-Verlag, Berlin Heidelberg.	2010

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

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

1. Subject Code: **CYN-904** Course Title: **Advanced Physical Chemistry**
2. Contact Hours: **L: 03 T: 0 P: 0**
3. Examination Duration (Hrs.): **Theory 3 Practical 0**
4. Relative Weightage: **CWS 20-30 PRS 0 MTE 20-30 ETE 40-60 PRE 0**
5. Credits: **3** 6. Semester: **Autumn/Spring** 7. Subject Area: **PEC**
8. Pre-requisite: **NIL**
9. Objective: To familiarise the students with recent topics required for physical chemistry research
10. Details of the Course:

S. No.	Contents	Contact Hours
1.	Quantum Mechanics: Brief review of the postulates and various models, Hydrogen like and many electron systems, Slater determinants for ground and excited states of atoms. approximation methods, Hartree-Fock methods, Electron correlation and post Hartree-Fock methods.	7
2.	Density Functional Theory: Electron density and hole functions, The Hohenberg-Kohn theorems, the Kohn-Sham approach, exchange-correlation functionals	7
3.	Statistical Thermodynamics: The statistical method and ensembles, microcanonical ensemble, canonical ensemble, generalized ensembles, connection of ensemble formalisms to thermodynamics, Fermi-Dirac and Bose-Einstein statistics, phase space and Liouville equation, non-equilibrium statistical mechanics: affinities and fluxes, Onsager's regression hypothesis, time correlation functions, response functions.	14
4.	Spectroscopy: Phenomenological treatment of absorption, emission, and scattering. Einstein coefficients, spectral lineshapes, and Principles of laser emission. Time dependent perturbation theory, transition probabilities – Fermi Golden Rule, Finite lifetime of states. Rotational spectroscopy: fundamentals of rotational spectra of diatomic molecules and polyatomic molecules: spherical, symmetric, and asymmetric tops. Vibrational spectroscopy: vibration of diatomic molecules, harmonic and anharmonic oscillator, vibration of polyatomic molecules. Normal modes and group theory. Fermi interactions, vibrational angular momentum, Coriolis perturbations and inversion doubling. Electronic spectroscopy of molecules: electronic absorption spectra of diatomic molecules. Molecular orbitals and term symbols. Dissociation and pre-dissociation in the spectra of diatomic. Introduction to non-linear spectroscopy: two-photon and higher order processes and their applications	14
Total		42

11. Suggested Books

S. No.	Name of Authors /Books/Publishers	Year of Publication/ Reprint
1.	Schatz, G. C., Ratner M. A. "Quantum mechanics in chemistry", Prentice Hall	2002
2.	Szabo, A., Ostlund, N. S., "Modern quantum chemistry", 1 st Revised Edn, Dover Publishers.	2008

3	Cramer, C. J., "Essentials of computational chemistry", 2nd ed., John Wiley & Sons Ltd, West Sussex, England.	2002
4.	W. Koch, Holthausen, M. C., "A chemist's guide to density functional theory", 2nd ed., Wiley-VCH Verlag GmbH, Weinheim, Germany	2001
5.	McQuarrie, D. A., "Statistical mechanics", 1 st Ed., Viva Books.	2011
6.	Callen, H. B., "Thermodynamics and an introduction to thermostatistics", 2ed Ed, Wiley.	2006
7.	Chandler, D., "Introduction to modern statistical mechanics", Oxford University Press, Cambridge.	1987
8.	Bernath, P. F., "Spectra of atoms and molecules", Oxford University Press, Cambridge	2005
9.	Hollas, J. M., "Modern spectroscopy", Wiley.	2003
10.	Boyd, R. W., "Nonlinear optics", Academic Press	2009

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: **CHEMISTRY**

1. Subject Code: **CYN-905** Course Title: **Spectroscopic Methods of Structural Elucidation**

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

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

4. Relative Weight: **CWS: 20-30 PRS: 0 MTE: 25-30 ETE: 40-60 PRE: 0**

5. Credits: **4** 6. Semester: **Autumn/Spring** 7. Subject Area: **PEC**

8. Pre-requisite: **NIL**

9. Objective: To provide training in the elucidation of molecular structures using spectroscopic methods.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	Electronic Spectroscopy: Absorption, electronic transitions in inorganic and organic molecules, charge transfer transitions in organic and inorganic molecules, LMCT and MLCT, d-d transitions, Woodward-Fieser rules for alkenes, Woodward rules for enones and arenes, reflectance spectroscopic techniques.	6
2.	Emission Spectroscopy: Fluorescence, delayed fluorescence (TADF & TFDF), fluorescence quantum yield, lifetime, Stokes shift, solvent effects, types of quenching with kinetics, energy transfer mechanisms, electron transfer mechanisms, inter-system crossing, phosphorescence, aggregation-induced emission, photochromism, photocatalysis, photodynamic therapy, light-emitting cells.	10
3.	IR and Raman Spectroscopy: Active modes of vibrations, survey of functional groups in organic and inorganic compounds, effect of isotopic substitution, conjugation and symmetry; ATR and DRIFTS techniques; Raman	8
4.	Nuclear Magnetic Resonance Spectroscopy: Features of ¹ H NMR spectrum, chemical shifts, spin-spin couplings, coupling constants, dependence of J on dihedral angle, analysis of first order spectra and complex multiplets, chemical and magnetic equivalence and second order effects, OH/NH and dynamic processes, off-resonance decoupling, ¹³ C and other heteronuclei NMR spectra, NOE effects, chemical shift reagents, correlation spectroscopy, NMR of paramagnetic compounds, solid state NMR, simulation of NMR.	12
5.	Electron Spin Resonance Spectroscopy: Line shapes, isotropic and anisotropic interactions, theory of g-factors & hyperfine interactions, features of EPR spectra of metal complexes, structural information from EPR spectra of complexes, simulation of EPR.	6
Total		42

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication /Reprint
1.	Pavia, D. L., Lampman, G.M., Kriz, G. S., "Introduction to Spectroscopy", 5 th Ed., Cengage Learning India Private Limited, New Delhi.	2015
2.	Kemp, W., "Organic spectroscopy", 3 rd Ed, Macmillan, New York.	2011
3.	Crews, P., Rodríguez, J., Jaspars, M., "Organic structure analysis", 2 nd Ed, Oxford University Press, Oxford.	2010
4.	Williams D. H., Flemming, I., "Spectroscopic methods in organic chemistry" , 6 th Ed, Mc Graw Hill.	2011
5.	Silverstein, R. M., Webster, F. X., Kiemle, D. J., Bryce, D. L., Spectrometric identification of organic compounds", 8 th Ed, Wiley.	2014
6.	Weil, J. A., Bolton, J. R., "Electron paramagnetic resonance: Elementary theory and practical applications", 2 nd Ed, John Wiley & Sons Inc.	2007