DEPARTMENT OF CHEMISTRY

NATIONAL INSTITUTE OF TECHNOLOGY SRINAGAR

J&K-190006

.....

Ph.D. Chemistry

Revised Curriculum and Syllabi
(w.e.f. Autumn-2023)

REVISED CURRICULUM FOR PhD PROGRAM IN CHEMISTRY

.....

(2022)

Annexure-I

Programme Structure for PhD Course Work in Chemistry (Autumn-2023)

S. No.	Course Code	Course Name	L	T	P	C
A.	**Compulsory Course**					
1.	PHDCYT-601	Research Methodology	4	0	0	4
B.	**Specialization/Elective Courses (Choose Any Two)**					
2.	PHDCYT-602	Advanced Analytical Chemistry	3	0	0	3
3.	PHDCYT-603	Advanced Inorganic Chemistry	3	0	0	3
4.	PHDCYT-604	Advanced Organic Chemistry	3	0	0	3
5.	PHDCYT-605	Advanced Physical Chemistry	3	0	0	3
6.	PHDCYT-606	Biomass, Biofuels and Biorefinery	3	0	0	3
7.	PHDCYT-607	Biopolymers and Hydrogels	3	0	0	3
8.	PHDCYT-608	Characterization Techniques in Chemistry	3	0	0	3
9.	PHDCYT-609	Chemistry of Advanced Materials	3	0	0	3
10.	PHDCYT-610	Environmental Chemistry	3	0	0	3
11.	PHDCYT-611	Material's Electrochemistry	3	0	0	3
12.	PHDCYT-612	Modern Methods of Electronic Structures Elucidation	3	0	0	3
13.	PHDCYT-613	Natural Products Chemistry	3	0	0	3
14.	PHDCYT-614	Supramolecular Chemistry and Catalysis	3	0	0	3
15.	PHDCYT-615	Synthesis and Properties of Nanomaterials	3	0	0	3
C.	**Total Credits Required for PhD Chemistry Programme**		**4 + 6 = 10**			

Course Instructor (s) for PhD Programme in Chemistry (Autumn-2023)

S. No.	Course Code	Course Name	Course Instructor
1.	PHDCYT-601	Research Methodology	Dr Jignesh V. Rohit
2.	PHDCYT-602	Advanced Analytical Chemistry	Dr Mohammad Aslam
3.	PHDCYT-603	Advanced Inorganic Chemistry	Prof Hamida Chisti
4.	PHDCYT-604	Advanced Organic Chemistry	Dr Ravi Kumar
5.	PHDCYT-605	Advanced Physical Chemistry	Dr Shrikant Shivaji Maktedar
6.	PHDCYT-606	Biomass, Biofuels and Biorefinery	Dr Mohammad Aslam
7.	PHDCYT-607	Biopolymers and Hydrogels	Prof Kowsar Majid
8.	PHDCYT-608	Characterization Techniques in Chemistry	Prof Kowsar Majid
9.	PHDCYT-609	Chemistry of Advanced Materials	Dr Shrikant Shivaji Maktedar
10.	PHDCYT-610	Environmental Chemistry	Prof S. A. Shah
11.	PHDCYT-611	Material's Electrochemistry	Dr Shrikant Shivaji Maktedar
12.	PHDCYT-612	Modern Methods of Electronic Structural Elucidation	Prof Kowsar Majid
13.	PHDCYT-613	Natural Products Chemistry	Prof J. A. Banday
14.	PHDCYT-614	Supramolecular Chemistry and Catalysis	Prof Kowsar Majid
15.	PHDCYT-615	Synthesis and Properties of Nanomaterials	Prof Kowsar Majid

Subject: Subject: Research Methodology (Code: PHDCYT-601)	Syllabus for Ph. D Course Work (Compulsory Course)		Total Course Credit: 4		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	4	0	0
Course Instructor (s)	Dr Jignesh V. Rohit				

Course Objective	To impart the knowledge and awareness of research methodology for real-time contribution during an execution of research practices.
Course Outcomes (COs)	
CO1	To understand the basic concepts of research methodology, research problem and literature review.
CO2	To learn fundamentals of research design and research report writing.
CO3	To acquire knowledge of Statistics and apply it to examine research data.
CO4	To lean application of computers in analyzing research data.
MODULE-I	**Introduction of Research Methodology, Defining the research problem and Literature review [10L]** Introduction of research methodology: Meaning, Objectives, Types, Approaches and Significance of Research, Research Methods versus Methodology, Research and Scientific Method, Research Process, Criteria of Good Research Defining the research problem: Meaning and Selection of the Problem, Necessity of Defining the Problem, Technique Involved in Defining a Problem Literature review: Searching of the existing literature, Reviewing the selected literature, Developing theoretical and conceptual framework, Clarity about research problem, contextualize findings
MODULE-II	**Research design and Report writing [10L]** Research design: Concepts and types of Research Design, Need of Research Design, Features of a Good Design, Basic Principles of Experimental Designs, Important Experimental Designs Report writing: Significance of Report Writing , Different Steps in Writing Report, Layout of the Research Report , Types of Reports, Oral Presentation, Mechanics of Writing a Research Report, Precautions for Writing Research Reports
MODULE-III	**Statistical data analysis [10L]** Errors, classification of errors and their minimization; absolute, relative, determinate and indeterminate errors, accuracy and precision, methods of expressing accuracy and precision, mean and standard deviation, confidence

	intervals, statistical tests of data (the F test, the t test, Q test, ANOVA), Concepts and difference between LOD and LOQ
MODULE-IV	**Computer based data analysis techniques [10L]** Origin and Excel spreadsheets for data analysis: least square and successive approximation, correlation and regression-linear and non-linear, multiple variable matrix and its analysis, drawing of good fit lines, slopes, correlation coefficient and their significance.

Recommended Books:

1. Prathapan K., Research Methodology for Scientific Research, Dreamtech Press, 1st edition, 2019.
2. Kothari C.R., Garg G., Research Methodology: Methods and Techniques, New Age International Publisher, 4th Edition, 2019.
3. Christian G.D., Dasgupta P.K., Schug. K.A., Analytical Chemistry, Wiley-VCH Publication, 7th edition, 2014.
4. Kumari R., Computers and their Applications to Chemistry, Alpha Science International Ltd, 2nd edition, 2005.
5. Marder M.P., Research Methods for Science, Cambridge India, 1st edition, 2011.
6. Kumar R., Research Methodology: A step by step guide for beginners, Sage Publication, 3rd Edition, 2011.
7. Skoog D.A., West D.M., Holler F.J., Crounch S.R., Fundamentals of Analytical Chemistry, Cengage Learning India Pvt. Ltd., 6th edition, 2009.
8. Wilson S., Chemistry by Computer: An Overview of the Applications of Computers in Chemistry, Plenum Publishing Corporation, 1st edition, 2011.

Subject: Advanced Analytical Chemistry (Code-PHDCYT-602)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Dr Mohammad Aslam				

Course Objective	The course has been designed to enable the PhD students to learn various advanced analytical techniques that would be applied in all frontier areas of research and development.
Course Outcomes (COs)	
CO1	To acquire the knowledge about the various thermal methods like TGA, DTG, DTA, DSC and their applications to material science.
CO2	To get knowledge of X-ray methods (XRD/XRF/XPS/AES) for the analysis of surface of solid materials.
CO3	To gain knowledge about electron microscopy (i.e., SEM and TEM) to characterize the surface of solid materials.
MODULE-I	**Thermal Methods of Analysis [10 L]** Introduction to thermal methods, classification of thermal methods, Thermogravimetric analysis, apparatus, methodology, applications; derivative thermogravimetry, instrumentation, methodology, applications; differential thermal analysis, apparatus, methodology, applications; differential scanning calorimetry; instrumentation, methodology and applications. Comparative study of TGA, DTA and DSC. Interpretation of various thermograms of important compounds e.g., silver nitrate, calcium oxalate monohydrate, magnesium oxalate dihydrate. Thermogravimetric analysis of dolomite and calcite samples and their purity analysis. Good praxis for thermal experiments, applications of thermal methods in material science.
MODULE-II	**X-ray Methods of Analysis [10 L]** Introduction to X-ray methods, generation of X-rays, X-ray Diffraction; principle, theory, instrumentation, chemical analysis with X-ray diffraction and applications. X-ray Fluorescence; principle, instrumentation, chemical analysis and applications. X-Ray photoelectron spectroscopy (XPS/ESCA); principle, chemical shifts as a function of oxidation states, instrumentation, applications;

	Auger electron spectroscopy (AES); principle, instrumentation-radiation source, energy analyzer, detector, auxiliary system; applications.
MODULE-III	**Electron Microscopy for Surface Analysis [10 L]** Introduction to electron microscopy, classifications of electron microscopy, scanning electron microscopy (SEM); fundamentals, secondary electrons, backscattered electrons, sample preparation, instrumentation, applications. Transmission electron microscopy (TEM); Introduction, basic theory, electron gun, electromagnetic lens, condenser lens, objective lens, projector lenses, imaging, operating parameters-magnification, resolution, depth of field; sample preparation, specimen orientation and manipulation; applications.

Recommended Books:

1. Harvey D., Modern Analytical Chemistry, 2000, McGraw Hill Education, New York.
2. Skoog D., Holler F., Crouch S., Principles of Instrumental Analysis, 7th Edition 2017, Brooks/Cole Publishers.
3. McNair H. M., Miller J. M., Snow N. H., Basic Gas Chromatography, 3rd Edition, 2019, Willey.
4. Echlin P., Fiori C.E., Goldstein J., Joy D. C., Newbury D. E., Advanced Scanning Electron Microscopy and X-Ray Microanalysis, 2013, Springer.
5. Williams D. B., Carter C. B., Transmission Electron Microscopy: A Textbook for Materials Science, 2nd Edition, 2009, Springer.
6. Kaur H., Instrumental Methods of Chemical Analysis (Analytical Chemistry), 2012, Pragati Prakashan, Meerut.
7. Chatwal G. R., Anand S. K., Instrumental Methods of Chemical Analysis, 5th Edition, 2019, Himalya Publishing House, New Delhi.

Subject: Advanced Inorganic Chemistry (Code-PHDCYT-603)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof. Hamida Chisti				

Course Objective	To Understand molecular chemistry, chemical bonding, structure and reactions of Coordination and Organometallic compounds, inorganic reaction mechanism, Bioinorganic chemistry.
Course Outcomes (COs)	
CO1	To learn about the structure, bonding and reactions in Coordination compounds.
CO2	To learn about the bonding, various reaction pathways and to analyze the structure by electronic spectra in Organometallic compounds.
CO3	To learn about the role of metal ions in Biochemistry, and to explain the importance of minerals in life.
MODULE-I	**Coordination Chemistry [10 L]** Theories of electronic Structure: Terminology and Historical background of VBT and CFT. Ligand Field Theory: Molecular Orbitals for octahedral complexes, Orbital splitting and electron spin, ligand Field stabilization energy, pi bonding, square planer complexes, tetrahedral complexes. Angular overlap: Sigma-donor interactions, pi acceptor interactions, pi donor interactions, types of ligands and the spectrochemical series. The Jahn Teller effect: Octahedral and Tetrahedral Complexes.
MODULE-II	**Organo-metallic Reactions and Catalysis [10 L]** An introduction to Organometallic compounds, Metal Carbonyls: classification of metal carbonyls, bonding in metal carbonyls. Reactions involving gain or loss of ligands: Ligand dissociation and substitution. Spectral properties of M-H bond (^{1}H NMR), ^{31}P NMR, ^{13}C NMR and ESR (Electron Spin Resonance) Spectroscopy. Metal Nitrosyls. Cluster Compounds, The Isolobal Analogy. Metal Carbene complexes, Metal Carbyne complexes, Metal Allyl complexes, and Metal Buta-1,3-diene complexes. Cyclic polyene complexes. Catalysis: Catalytic cycles, Application of organometallic compounds as homogenous catalysts, Hydrogenation of Alkenes (Wilkinson's Catalyst), Oxo process, Wacker process,

	and Cativa process. Heterogenous Catalysis: Alkene polymerization (Ziegler Natta catalyst). Coupling Reactions.
MODULE-III	**Bioinorganic Chemistry [10 L]** Role of metal ions in Metalloenzymes, Metalloporphyrin's, Phthalocyanines, Chlorophyll and Cytochromes etc. Biochemistry of Iron and its role in hemoglobin and myoglobin. Essential and trace elements in biological systems. Biological role of elements like Zn, Cu, Ca, Mg, Na and K. Complexation of some Antibiotics and related compounds like Valinomycin, Oxytetracycline and D-Penicillamine.

Recommended Books:

1. Inorganic Chemistry, James E. Huheey, Pearson. 4th Edn.
2. Inorganic Chemistry, Gary L. Miessler, Donald A. Tarr, Pearson, Third Edn.
3. Inorganic Chemistry, F.A. Cotton, Wiley, 6th Edn.
4. Inorganic Chemistry, Weller and Armstrong, Oxford, 6th Edn.
5. Inorganic Chemistry, J. D. Lee, Wiley, 5thEdn.
6. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.

Subject: Advanced Organic Chemistry (PHDCYT-604)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Dr Ravi Kumar				

Course Objective	The course has been designed to enable the students to learn the retrosynthesis, reagents in organic synthesis and spectroscopic analysis of organic molecules.
Course Outcomes (COs)	
CO1	To learn the various reagents employed in modern organic synthesis.
CO2	To learn retrosynthetic approach in the art of modern organic synthesis.
CO3	To familiarize the students with the organic structure determination methods involving spectroscopy.
MODULE-I	**Reagents in Organic Synthesis [10 L]** Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, Lithium diisopropylamide (LDA), Diisobutylaluminium hydride (DIBAL-H), 1,3-dithiane (reactivity Umpoloung), Trimethylsilyl iodide, tri-n-butyltin hydride, osmium tetroxide, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), selenium dioxide, Phase transfer catalysts, crown ethers and Wilkinson's catalyst
MODULE-II	**Organic Synthesis [10 L]** Retrosynthetic analysis: Basic principles and terminology of retrosynthesis, guidelines, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, important strategies of retrosynthesis, important functional group interconversions. Protection and deprotection of functional groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds, chemo- and regioselective protection and deprotection.
MODULE-III	**Spectroscopic Methods in Organic Chemistry [10 L]** Applications of UV spectroscopy to Conjugated dines, trienes, unsaturated carbonyl compounds and aromatic compounds. Nuclear Magnetic Resonance Spectroscopy (Proton and Carbon -13 NMR) The measurement of spectra: the chemical shift: the intensity of NMR signals and integration factors affecting the chemical shifts, first order coupling: some simple ^{1}H-^{1}H splitting patterns: the

	magnitude of ^{1}H-^{1}H coupling constants. Mass Spectrometry: Principle, instrumentation and techniques. Fragmentation pattern of some representative class of compounds; Hydrocarbons, Alcohols, Ketones, Phenols and Carboxylic acids.

Recommended Books:

1. Advanced Organic Chemistry, 7th Ed. - Smith, M. B., March (Wiley – 2016)
2. Organic synthesis: The disconnection approach, 2nd Ed., - Warren, S., and Wyatt, P. (Wiley – 2008)
3. Protective Groups in Organic Synthesis Greene, T.W. (Wiley- 1999)
4. Organic Spectroscopy 3rd Ed., - Kemp, W. (Macmillan -1994)
5. Spectroscopy of organic compounds, 6th Ed., Kalsi, P. S. (New Age International – 2004)

Subject: Advanced Physical Chemistry (PHDCYT-605)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Dr Shrikant Shivaji Maktedar				

Course Objective	To learn advanced concepts in physical chemistry with spectroscopic techniques for structural elucidation
Course Outcomes (COs)	
CO1	To learn and understand the several techniques of characterization
CO2	To learn the surface chemistry with kinetic processes
CO3	To understand interfacial electrochemistry and catalytic processes
MODULE-I	**Molecular Spectroscopy [10L]** Molecular spectra, Rotational or microwave spectra, Rotational spectra of polyatomic molecules, Stark effect in microwave spectra, Application of microwave spectra, Vibrational spectra, Rotation vibration spectra: Infrared spectra, Vibrational spectra of polyatomic molecules, Raman spectroscopy, Electronic spectra, Charge transfer spectra, Electronic spectra of transition metal ions and conjugated molecules, Electron spin resonance spectra, ESR spectrum of unpaired electrons, Hyperfine structure in ESR spectra, The g-factor, Application of ESR spectra, Photoelectron spectroscopy
MODULE-II	**Surface Chemistry & Kinetics [10L]** Adsorption by solids, Chemisorption, Adsorption of gases by solids, Factors influencing adsorption, Freundlich and Langmuir adsorption isotherm, BET theory, Adsorption from solutions, Gibbs adsorption isotherm, Rate equation, Order of reaction, Integration of rate expression, Zero, First, Second and Third order reaction, Half-life time of the reaction, Method for determining order of reaction, order and molecularity of simple reactions
MODULE-III	**Electrified Interfaces [10L]** Quantitative and thermodynamic treatment of electrified interfaces, determination of surface excess, structure of electrified interfaces, Helmholtz-Perrin model, Gouy-Chapman diffuse charge model of double layer, Stern model, Structure of semiconductor interfaces, Garrett-Brattain space charge inside intrinsic semiconductor, electrocatalysis, mechanism of electrocatalysis, volcanoes, Kinetics of electrode reaction, Butler-Volmer equation, Diffusion

	overpotential, Irreversible electrode processes, overvoltage.

Recommended Books:

1. P Atkins and J de Paula, Physical Chemistry
2. Puri, Sharma and Pathania, Principles of Physical Chemistry

Subject: Biomass, Biofuels and Biorefinery (Code-PHDCYT-606)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Dr Mohammad Aslam				

Course Objective	This course is aimed at dissemination of important information of biomass and biorefinery to enable students to acquire knowledge on cutting-edge technologies for conversion of various biomass feedstock to biofuels production using biorefinery concept for sustainable developments.
Course Outcomes (COs)	
CO1	To get knowledge about biomass resource assessment and their global potential and advanced biofuels derived from them.
CO2	To understand both the biochemical and thermochemical conversion processes for the production of biofuels and value-added bio-products.
CO3	To understand the fundamentals of biorefinery and integrated biorefinery concepts including first, second and third generation biorefineries.
MODULE-I	**Biomass Resources Assessment [10 L]** Global energy requirements, depletion of conventional energy resources and their impact on the environment, need & availability of renewable energy resources, bioenergy resources, types and availability of biomass resources, World's and India's bioenergy potential, biofuels policy-2018, biomass resources and classification, physio-chemical characteristics of biomass, biomass characterization, proximate/ultimate analysis, compositional analysis, heating value, thermogravimetric, differential thermal analyses. Modern concepts of biofuels & classification, physio-chemical characteristics of solid, liquid and gaseous biofuels and their composition, basic understanding of various fuel properties of solid, liquid and gaseous biofuels.
MODULE-II	**Biomass Conversion Processes [10 L]** Biochemical conversion processes, fermentation, anaerobic/aerobic processes, thermochemical conversion processes, combustion, gasification, pyrolysis, hydrothermal liquefaction and Integrated hybrid conversion processes for energy generation applications. Liquid biofuels production process and technology, bioethanol and biobutanol production from lignocelluloses, waste

	material, crop residue, sugar and starch. Biodiesel and green diesel production from second and third generation biomass feedstocks. Production of green hydrogen from biomass feedstocks. Production of biofuels, bioproducts and chemicals from biomass and wastes. Life cycle and technoeconomic analysis of biofuel production.
MODULE-III	**Biorefinery Concept [10 L]** Introduction to bio-refinery concept, different types of bio-refineries; first, second and third generation biorefineries, examples of biorefinery, challenge and opportunities. Biofuels, bioproducts and platform molecules derived from lignocellulosic biomass using biorefinery concept, second generation liquid biomass based biorefinery, algal biorefinery, co-feedstocks for biorefinery, by-products derived from second/third generation biorefineries, integrated biorefinery approach. A comparative analysis of conventional refinery and biorefinery. Current status and future outlook of second/third generation biorefineries, case studies.

Recommended Books:

1. Sahay S., Handbook of Biofuels, 1st Edition, 2021, Elsevier Publishers, USA.
2. Dahiya A., Bioenergy: Biomass to Biofuels, 2014, Academic Press, USA.
3. Luque R., Lin C. S. K., Wilson K., Clark J., Handbook of Biofuels Production: Processes and Technologies, 2nd Edition, 2016, Elsevier Publishers, USA.
4. Konur O., Bioenergy and Biofuels, 2018, CRC Press, UK
5. Oyanedel J. B., Schmidt J. E., Biorefinery: Integrated Sustainable Processes for Biomass Conversion to Biomaterials, Biofuels, and Fertilizers, 2019, Springer.

Subject: Biopolymers and Hydrogels (Code- PHDCYT-607)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof. Kowsar Majid				

Course Objective	The course is aimed at acquainting students with basic knowhow of Biopolymers with special emphasis on Hydrogels, their characterization and modern-day applications.
Course Outcomes (COs)	
CO1	To acquire the knowledge of biopolymers, bio-based composites, and their mechanical properties.
CO2	To learn fundamentals, synthesis and classification of hydrogels.
CO3	To get knowledge of swelling behavior of hydrogels, and their advanced applications.
MODULE-I	**Fundamentals of Biopolymers [10 L]** Definition of biopolymers and types of biopolymers, Description of certain biopolymers like starch, cellulose, chitosan, gelatin, alginate, keratin, fatty acids, lipids, aliphatic polyesters (PLA, PHB), Cellulose derivatives and cellulose regenerating processes, Bio based composites, natural biodegradable polymer, synthetic biodegradable polymer and modified naturally biodegradable polymer, Concept of biocompatibility and responsiveness, Technically important forms of polymers (Hydrogel, bioceramics, bioelastomers and membranes), Mechanical properties (elasticity, yield stress, ductility, toughness, strength, fatigue, hardness and wear resistance) of biomaterials.
MODULE-II	**Fundamentals and Synthesis of Hydrogels [10 L]** Introduction to hydrogel and brief historical overview, Classification of hydrogels based on origin, type of interaction, and ionic/non-ionic characteristics, Different types of gel forming techniques (Physically and chemically cross-linked hydrogels), Introduction to stimuli responsive hydrogels and their types.
MODULE-III	**Characterization and applications of Hydrogels [10 L]** Evaluation of swelling behaviors of hydrogels (Swelling capacity and water retention capacity) and kinetic analysis, Effect of pH, ionic strength and

	temperature on swelling properties of hydrogels, Relationship between morphology and swelling properties, Mechanical and rheological properties of hydrogel, smart hydrogels, characterization of hydrogels, Applications of Hydrogels in adsorption, 3D printing, shape memory materials, drug release and other biomedical applications.

Recommended Books:

1. Gowarikar, V. R., 1997, Polymer Science, New Age International Pvt. Ltd., New Delhi.
2. Odian, G., 2001, Principles of Polymerization, John Wiley & Sons, New York.
3. Cantor, C.R., and Schimmel, P.R., 1980, Biophysical Chemistry, Freeman, Oxford.
4. Michael Niaounakis, 2015, Biopolymers: Applications and Trends, William Andrew Publication, New York.
5. Campbell D. and White J.R., 1989, Polymer Characterization: Physical Techniques, Chapman & Hall, London.
6. https://nptel.ac.in/courses/102/106/102106057/
7. https://iopscience.iop.org/article/10.1088/1742-6596/3/1/004/pdf
8. https://www.chemistrylearner.com/biopolymer.html

Subject: Characterization Techniques in Chemistry (Code- PHDCYT-608)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof. Kowsar Majid				

Course Objective	The course has been designed to enable the students to learn the fundamentals, instrumentation, and data interpretation of various material characterization techniques.
Course Outcomes (COs)	
CO1	To learn and apply various Spectroscopic and Thermo analytical methods.
CO2	To learn material surface characterization techniques and their interpretation.
CO3	To gain knowledge of various mechanical and electrical properties of nanomaterials and their evaluation through different techniques.
MODULE-I	**Spectroscopic Characterization [10 L]** Basic theory, instrumentation and analytical applications of the following physical methods: Spectroscopic techniques (NMR, ESR, MS (EI, FAB, MALDI-TOF), IR, UV-Vis, Emission and Absorption Spectroscopy, X-ray diffraction (single crystal & powder), Thermo analytical methods (TGA, DSC, DTA). Application of these techniques for characterization of samples.
MODULE-II	**Surface Characterization [10 L]** Basic theory, instrumentation and analytical applications of the following physical methods: microscopic methods (Polarized optical microscope, SEM, TEM, AFM), Surface Properties (XPS, BET).
MODULE-III	**Mechanical and Electrical Characterization [10 L]** Study of mechanical properties through viscometry and Rheometry. Study of electrical properties through Cyclic Voltammetry, Four-Point Probe, and Thermal Probe techniques.

Recommended Books:

1. R.M. Silverstein and F.X. Webster, 2003, Spectroscopic Identification of Organic Compounds, 6th Edition. John Wiley, New York.

2. J.R. Dyer, 1978, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, New Delhi.
3. J.M. Hollas, 2004, Modern Spectroscopy, 4th Edition, John Wiley and Sons, Chichester.
4. C.N. Banwell and E.M. Mc Cash, 1994, Fundamentals of Molecular Spectroscopy, 4th Edition, Tata McGraw Hill, New Delhi.
5. R.S. Drago, 1992, Physical Methods in Chemistry, International Edition, Affiliated East-West Press, New Delhi.
6. D.A. Skoog, F.J. Holler and T.A. Nieman, 1998, Principles of Instrumental Analysis, 5th Edition, Harcourt Brace & Company, Florida.
7. H.A. Strobel, 1973, Chemical Instrumentation – A Systematic Approach, 2nd Edition, Addison Wesley, Boston.
8. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, 1976, Modern Methods of Chemical Analysis, 2nd Edition. John Wiley, New York.

Subject: Chemistry of Advanced Materials (Code- PHDCYT-609)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Dr Shrikant Shivaji Maktedar				

Course Objective	To learn electrochemical techniques and structural elucidation of advanced materials for energy, environment and healthcare application
Course Outcomes (COs)	
CO1	To learn and understand structure, properties and applications of carbon nanostructures
CO2	To learn and understand the properties of emerging 2-D materials
CO3	To learn and understand electron transfer kinetics
MODULE-I	**Carbon Nanostructures [10L]** Classification of carbon allotropes, Natural allotropes of carbon and their properties, Artificial allotropes of carbon and their properties, Physical and chemical synthesis methods of fullerene, carbon nanotube, graphene, covalent and non-covalent functionalization of graphene, carbon-based materials for energy, environment and healthcare applications.
MODULE-II	**Advanced 2D Materials [10L]** Classification, structure and properties of advanced 2-D materials such as Graphene, Mxenes, MoS_2, h-BN, g-C_3N_4 etc. with methods of structural characterization and their potential applications.
MODULE-III	**Hydrodynamic Electrochemistry [10L]** Kinetics of electron transfer, current overpotential curve, Charge transfer resistance, Multistep mechanism, Kinetics of hydrogen evolution, Electron transfer rate from voltammetry, One electron processes, Two electron processes, Criteria for reversibility, Faradic impedance.

Recommended Books:

1. Christopher M.A. Brett, Ana Maria Oliveria Brett, Electrochemistry: Principles, Methods and Applications, Oxford university press.
2. Philip H Rieger, Electrochemistry, Second edition, Chapmann & Hall publishing.

Subject: Environmental Chemistry (Code- PHDCYT-610)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof. S. A. Shah				

Course Objective	The course has been designed to enable the students to learn about structure of environment, its pollution, analysis and control.
Course Outcomes (COs)	
CO1	To understand different segments of Environment
CO2	To Learn about various types of pollution and factors responsible.
CO3	To learn about pollution status and analysis
MODULE-I	**Environmental Segments [10 L]** Atmosphere: Composition and Structure. Hydrosphere: Chemical Composition, Aquatic Pollution. Lithosphere: Nature, Composition of Soil and Soil Profile.
MODULE-II	**Environmental Pollution [10 L]** Air Pollution: Smog and Photochemical Smog and its effects. Water Pollution: Pollution, Water Quality Parameters and its control. Soil Pollution: Soil erosion and factors responsible for erosion, its control. Soil degradation and its sources. Industrial Pollutions: Cement, Drug, Thermal Power Plants.
MODULE-III	**Pollution Status and Analysis [10 L]** Air Pollution: Analytical methods via continuous monitoring instruments. Water Pollution: Determination of water quality parameters by analytical methods. Soil Pollution: Acid – Base and ion – exchange methods.

Recommended Books:

1. Environmental chemistry; A. K. De; Wilay Eastern; 1995.
2. Environmental chemistry; S. E. Manahan; Lewis Publishers; 2000
3. Environmental Sciences; Dr. R.J. Chhatwal; 2nd Revised Edition 2011.
4. Environmental Pollution analysis; S. M. Khopkar; Wiley Eastern.

Subject: Material's Electrochemistry (Code- PHDCYT-611)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Dr Shrikant Shivaji Maktedar				

Course Objective	To learn electrochemical techniques and structural elucidation of advanced materials for energy, environment and healthcare application
Course Outcomes (COs)	
CO1	To learn and utilize electrochemical techniques
CO2	To learn the sophisticated methods of structural elucidation
CO3	Applications of advanced materials for energy, environment and healthcare
MODULE-I	**Electrochemistry & Catalysis [10L]** Hydrodynamic methods, Rotating disk electrode (RDE), Rotating ring disk electrode (RRDE), Transients at RDE & RRDE, Microkinetic analysis, Cyclic voltammetry (CV), Linear sweep voltammetry (LSV), Electrochemical impedance spectroscopy (EIS), Galvanostatic charge discharge (GCD), Tafel plot, Nyquist plot, Overpotential, Turn over frequency (TOF), Open circuit potential (OCP), Differential pulse voltammetry (DPV), with calculations and interpretation,
MODULE-II	**Structure & Properties of Advanced Materials [10L]** XRD, XPS, Raman, SSNMR, TEM, SAED, SEM, EDS, AFM, BET, TG-DTA, DSC, Contact angle, Rheology, UV-DRS, FTIR, PL, Tribological properties, GCMS, HPLC, with analysis.
MODULE-III	**Energy, Environment & Healthcare [10L]** Hydrogen evolution reaction (HER), Oxygen evolution reaction (OER), Oxygen reduction reaction (ORR), Nitrate reduction reaction (NRR), Carbon dioxide reduction reaction, Transient photocurrent, Dye degradation and heavy metal ion detection, Photo-electrocatalysis, Spectro-electrochemistry, Screen printed electrode (SPE), Molecularly imprinted polymers (MIP) for electrochemical biosensors, Biological assay.

Recommended Books:

1. Kissinger, Peter; William R. Heineman (1996-01-23). Laboratory Techniques in Electroanalytical Chemistry, Second Edition, Revised and Expanded (2 ed.). CRC.
2. Zoski, Cynthia G. (2007-02-07). Handbook of Electrochemistry. Elsevier Science.

Subject: Modern Methods of Electronic Structural Elucidation (Code- PHDCYT-612)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof Kowsar Majid				

Course Objective	The course has been designed to enable the students to learn the advanced quantum chemistry.
Course Outcomes (COs)	
CO1	To acquire the knowledge about the approximation methods in quantum chemistry.
CO2	To study multi-electron systems and learn Hartree-Fock approximation.
CO3	To gain knowledge of Density Functional theory.
MODULE-I	**Approximation Methods [10 L]** The variational method**,** Trial functions that depend linearly on variational parameters, Trial functions that depend non-linearly on variational parameters, Introduction to perturbation theory, First-order perturbation theory, Selection rules and time-depoendent perturbation theory.
MODULE-II	**Multi-electron systems and Hartree-Fock Approximation [10 L]** Many electron operators and wave functions, Born-Oppenheimer Approximation, Antisymmetry principle, Spin and space orbitals, Hartree product and Slater determinant wave functions. Hartree-Fock approximation, Minimal basis H_2 model, One and two electron integrals, Coloumb and exchange operators/integrals in light of minimal basis H_2 model. Roothan equations and their matrix form, Self-consistent procedure, Basis sets, Limitations of Harttree-Fock model, Electron correlation, Brief introduction to multi-determinant wave function methods (Configuration interaction and Coupled Cluster methods).
MODULE-III	**Introduction to Density Functional Theory [10 L]** Density Functional Theory: Electron density as basic variable**,** Hohenberg-Kohn theorems, Kohn-Sham approach, Orbitals and the non-interacting reference system, Kohn-Sham equations and potential. Exchange-Correlation energy in the Kohn-Sham scheme, Exchange-Correlation functional, Local density and local Spin-Density approximations, Generalized Gradient approximation, Hybrid

	functionals.

Recommended Books:

1. Ira. N. Levine, 2013, Quantum Chemistry, 7th Edn., Prentice Hall, New Delhi.
2. P. W. Atkins and R. S. Friedmann, 2008, Molecular Quantum Mechanics, 5th Edn. Oxford.
3. A. Szabo & N. S. Ostlund, 1996, Modern Quantum Chemistry Introduction to Advanced electronic structure theory, Macmillan, New York.
4. T. Helgaker, P. Jorgensen and J. Olsen, 2000, Molecular Electronic-Structure Theory, Wiley-VCH.
5. R.G. Parr and W. Yang, 1989, Density Functional Theory of Atoms and Molecules, Oxford.
6. W. Koch and M. C. Holthausen, 2001, A Chemist's Guide to Density Functional Theory, 2nd Edn., Wiley-VCH.

Subject: Natural Products Chemistry (Code- PHDCYT-613)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof. J. A. Banday				

Course Objective	The course has been designed to enable the students to learn the structure, isolation, characterization and biological activity of Natural Products.
Course Outcomes (COs)	
CO1	To familiarize the students with significance of natural products; their chemistry and synthesis
CO2	To learn various methods of isolation, characterization and importance of essential oils.
CO3	To impart the knowledge of determination of biological activity of organic molecules.
MODULE-I	**Natural Products [10 L]** Role of natural products in drug discovery, Natural products as drugs. Nomenclature, classification and characteristic chemical properties of coumarins, flavonoids, terpenoids, steroids and alkaloids. Biomimetic Synthesis, Total synthesis and semi-synthesis of Natural Products
MODULE-II	**Essential Oils [10 L]** Chemical composition, methods of isolation and characterization of essential oils. Identification of major constituents of essential oils isolated from various sources. Role of essential oils in perfumery/flavour industry and aroma therapy.
MODULE-III	**Bio-evaluation Studies [10 L]** Factors affecting bioactivity. Methods of evaluation of different biological activities of organic compounds. In vitro anticancer activity, laboratory based anti-oxidant activity, anti-microbial activity.

Recommended Books:

1. Organic Chemistry, Finar Vol. I & II, ELBS-Longman, 1975.
2. Principles of Medicinal Chemistry, William O. Foye, Verghese Publishing House, 1995.
3. Biosynthesis of Natural Products, J. D. Local: Mac Graw Hill, 1965.

4. Total Synthesis of Natural Products, Jie Jack Li and E.J. Corey, 2012, Springer.
5. Classics in Total Synthesis: Targets, Strategies, Methods, K.C. Nicolaou and E. J. Sorenson, 1996, Wiley-VCH.
6. Biomimetic Organic Synthesis: Erwan Poupon and Bastien Nay, 2011, Wiley-VCH.
7. Chemistry of Natural Products, 1st Edition, S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, 2008, Arosa Publishing House.

Subject: Supramolecular Chemistry & Catalysis (Code- PHDCYT-614)	Syllabus for PhD Course Work (Specialized/Elective Course)		Total Course Credit: 3		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof. Kowsar Majid				

Course Objective	The course aims at understanding the fundamentals of supramolecular chemistry, design of supramolecules, and their applications. The course also lays emphasis on homogenous catalysis and its industrial applications.
Course Outcomes (COs)	
CO1	To get basic knowledge of supramolecular chemistry.
CO2	To get acquainted with design, synthesis, properties, and applications of supramolecules.
CO3	To learn about homogenous catalysis, catalysis selectivity and industrial applications of homogenous catalysis.
MODULE-I	**Supramolecular Chemistry-I [10 L]** Concepts of Supramolecular Chemistry: Definition, Nature of supramolecular interactions, Host-guest interaction, Molecular recognition, Types of recognition. Cation-binding Hosts: Concepts, Cation receptors, Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, Selectivity of cation complexation, Macrocyclic and template effects. Anion-binding Hosts: Concepts, Anion host design, Anion receptors, Shape and selectivity, Cation hosts to anion hosts, pH effect. Neutral receptors: Clathrates, cavitands, cyclodextrins, cyclophanes.
MODULE-II	**Supramolecular Chemistry-II [10 L]** Self-assembly molecules: Design, synthesis and properties of the molecules, Self-assembling by H-bonding, Metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots. Applications of Supramolecular Chemistry: Rational Design, molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic. cyclodextrins as enzyme mimics, ion channel mimics, supramolecular reactivity and catalysis.
MODULE-III	**Homogeneous Catalysis [10 L]**

	Catalysis: Terminology in catalysis, TO(Turnover), TON (Turnover number), TOF (Turnover frequency), Sequences involved in a catalyzed reaction, other terms used in catalysis, enantioselectivity, stereoselectivity, chemo-selectivity, regioselectivity, Asymmetric synthesis using a catalyst. Hydroformylation: Importance, Cobalt catalyst for hydroformylation, Phosphine-modified cobalt catalysis, Rhodium-Phosphine catalyst, Factors affecting n/iso ratio of hydroformylation product, Enantioselective hydroformylation. Methanol Carbonylation and Olefin Oxidation: Monsanto process of conversion of methanol to acetic acid.

Recommended Books:

1. Ariga, Katsuhiko, Toyoki Kunitake, Supramolecular Chemistry - Fundamentals and Applications, Springer.
2. J.M. Lehn, Supramolecular Chemistry: Concepts and perspectives, Wiley VCH.
3. G. R. Desiraju, J. J. Vittal, A. Ramanan, Crystal Engineering, World Scientific.
4. E. R. T. Tiekink, J. Vittal, M. Zaworotko, 2010, Organic Crystal Engineering: Frontiers in Crystal Engineering, Wiley.
5. Edward R. T. Tiekink, Jagadese Vittal, 2005, Frontiers in Crystal Engineering, Wiley-VCH.
6. Asim K. Das, Mahua Das, 2005, An Introduction to Supramolecular Chemistry, CBS Publishers and Distributors Pvt Ltd.
7. Amabilino, D. B.; Smith, D. K.; Steed. J. W, Supramolecular materials, Chem. Soc. Rev., 2017, 46, 2404-2420
8. Huheey. E. Keiter, R. Keiter, 1983, Inorganic Chemistry, Addison-Wesley.
9. Gary L. Miessler, Donald A. Tarr, Inorganic Chemistry, Pearson.
10. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley.
11. B.D. Gupta & A.J. Elias, 2013, Organometallic Chemistry, University Press.

Subject: Synthesis and Properties of Nanomaterials (Code- PHDCYT-615)	**Syllabus for PhD Course Work (Specialized/Elective Course)**		**Total Course Credit: 3**		
Mid-Term	Internal Assessment	Final-Term	L	T	P
26 (Marks)	24 (Marks)	50 (Marks)	3	0	0
Course Instructor (s)	Prof Kowsar Majid				

Course Objective	The course has been designed to familiarize students with nanomaterial's design and applications.
Course Outcomes (COs)	
CO1	To learn the basics of nanomaterials and their classification based on their dimensionality and properties.
CO2	To acquire the knowledge of synthesis techniques of bulk nanostructured and nanocomposite materials.
CO3	To impart the knowledge of carbon-based nanomaterials and their applications with special emphasis on graphene, Carbon nanotube (CNT), and Fullerenes.
MODULE-I	**Nanomaterials-I** **[10 L]** Definition**,** Types of nanostructures, Properties and Applications**:** One dimensional, Two dimensional and Three dimensional nanostructured materials, Quantum Dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties, application as ferroelectric materials, coating, molecular electronics and nanoelectronics, biological and environmental, membrane based application, polymer based application, nanocatalysis, basic principle.
MODULE-II	**Nanomaterials-II** **[10 L]** Synthesis and preparation of Nanomaterials and Synthetic Techniques**:** Synthesis of bulk nanostructured materials - Sol Gel processing- bulk and nanocomposite materials - Grinding - high energy ball milling – injection moulding - extrusion - melt quenching and annealing, Self-assembly-Self Assembled Monolayers (SAM) - Vapour Liquid Solid (VLS) approach - Chemical Vapour Deposition (CVD), Hydrothermal and microwave method.
MODULE-III	**Nanomaterials-III** **[10 L]** Carbon nanostructures: Synthesis, separation and characterization of Fullerene and its derivatives, applications, toxicity. Carbon nanotube (CNT), structure,

	synthesis and functionalization of CNT, electronic, vibrational, mechanical and optical properties of CNT, applications. Graphene, structure, synthesis and functionalization of Graphene, Graphene composites, electronic applications of Graphene, Graphene Oxide. The environmental effects of carbon-based nanomaterials, Application of nanotechnology in Photodetectors, Nanophotonics, Nanoelectronic Devices, Biosensors, Naopolymers etc.

Recommended Books:

1. C. N. R. Rao, Achim Müller, A. K. Cheetham, 2004, Chemistry of nanomaterials: Synthesis, properties and applications, Wiley-VCH.
2. G. Schmidt, 2004, Nanoparticles: From theory to applications, Wiley-VCH.
3. E L Principe, P Gnauck, P Hoffrogge, 2005, Microscopy and Microanalysis, Cambridge University Press.
4. Juyoung Kim, 2012, Advances in Nanotechnology and the Environment, CRC Press, Taylor and Francis Group.
5. Brian R Eggins, 2002, Chemical Sensors and Biosensors, Wiley, New York.
6. J. Cooper & C. Tass, 2004, Biosensors: A Practical Approach, Oxford University Press.
7. C. S. Kumar, 2007, Nanomaterials for Biosensors, Wiley-VCH.
8. G.Cao, 2004, Naostructures and Nanomaterials: Synthesis, properties and applications, Imperical College Press.
9. W. Gaddand, D. Brenner, S. Lysherski, G. J. Infrate, 2002, Eds Handbook of nanoscience, Engg. and Technology, CRC Press.