

**DETAILED SYLLABUS OF COURSE WORK OF PH.D. PROGRAMME OF
DEPARTMENT OF CHEMISTRY, UNIVERSITY OF JAMMU**

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Course Title: **Research Methodology**

Course No.: **R-1**

Course Credits: **04**

Maximum Marks: **100**

Duration of Examination: **3 hrs**

Note: The candidates have to attempt five questions out of total nine, selecting at least one from each unit.

Thermal Techniques

Types of Techniques

Thermogravimetry (TG): Principle, Instrumentation, Application, Disadvantages.

Differential Thermal Analysis (DTA): Principle, Instrumentation, Application, Disadvantages.

Differential Scanning Calorimeter (DSC): Principle, Instrumentation, Application, Disadvantages, Comparison of DTA and DSC.

Thermo Mechanical Analysis (TMA) and Dynamic Mechanical Analysis (DMA): Principle, Instrumentation, Application, Disadvantages.

Electrochemical Techniques

Amperometry: Principle of amperometric titrations, Titration curves, Amperometric indicators, Instrumentation, Application, Biamperometric titrations.

Chronopotentiometry: Principle, Instrumentation, Cyclic voltammetry and stripping voltammetry.

Preparative Strategies: Ceramic method, Precursor method, Vapour phase transport methods, Electrochemical reduction methods, Microwave synthesis, The sol-gel method, Hydrothermal methods, Preparation of thin films: Chemical and electrochemical methods, Physical methods, Growth of single crystals, Dry high pressure methods.

Electron Microscopy

Scanning electron microscopy: Basic instrumentation, applications.

Transmission electron microscopy: Instrumentation, Basic theory, Electron gun, Electromagnetic lenses, Imaging, Operating parameters- Magnification, Resolution, Depth of field; Sample preparation, Specimen orientation and manipulation, Applications, Selected area electron diffraction.

Atomic force microscopy and Scanning tunneling microscopy.

Dynamic Light Scattering Studies: Principle, Theory and Methodology.

BET Surface Area Studies: Principle, Theory and Methodology.

Nuclear Magnetic Resonance (¹H and ¹³C)

Principles of NMR, Factors affecting chemical shift and spin-spin coupling, Improving the NMR spectra. The nuclear Overhauser effect. Recent developments in NMR, ¹H-¹H connectivity, 2D spectroscopy (COSY, APT, DEPT, INADEQUATE). Shift reagents, MRI.

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Mass Spectroscopy

Principle of ionization and ion-separation, Alternate modes of ion-formation (MALDI, ESI). Metastable peaks, fragmentation patterns, Intermolecular eliminations. Mass spectra of different classes of compounds.

Infrared Spectroscopy

Principle of IR spectroscopy, Instrumentation, Characteristic IR group frequencies, substitution pattern of the benzene rings, Fermi resonance, skeletal frequencies, analysis of IR spectra.

Ultra-violet Spectroscopy

Principle and applications, Origin of spectra and electronic transition, Reflectance spectroscopy, Spectra structure correlation, Woodward-Fieser rules, Steric inhibition of spectroscopy, Resonance and UV spectra, charge transfer spectra.

Applications: Applications of NMR, IR, UV and Mass spectroscopy for structural determination of Organic and Inorganic compounds.

BOOKS RECOMMENDED:

1. Principles and Practice of Analytical Chemistry by F.W. Fifield and D. Kealey; Blackwell Science Limited, 5th ed., 2000.
2. Instrumental Methods of Chemical Analysis by H. Kaur, Pragati Prakashan, 11th ed., 2016.
3. Solid State Chemistry and its Applications by A.R. West., John Wiley and Sons, 2004.
4. Solid State Chemistry: An introduction by Lesley Smart and Elaine Moore, CRC Press (Taylor and Francis Group), 2005.
5. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM and AEM by R.F. Egerton, Springer, 2016.
6. Atomic Force Spectroscopy by Peter Eaton and Paul West, Oxford University Press, 2010.
7. Solid State Chemistry: Techniques by A.K. Cheetham and Peter Day, Oxford University Press, 1987.
8. Scanning Probe Microscopy and Spectroscopy by Ronald Weisendanger, Cambridge University Press, 1994.
9. Spectroscopic Methods in Organic Chemistry by D.H. Williams and Ian Fleming, McGraw-Hill Higher Education, 2007.
10. Organic Spectroscopy by William Kemp, Palgrave Publishers, 2002.
11. Spectroscopic Identification of Organic Compounds by R.W. Silverstein, F.X. Webster and D.J. Kiemle, John Wiley and Sons, 2005.
12. Organic Spectroscopy: Principles and Applications by Jag Mohan, Narosa Publishing House, 2016.

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Course Title: **Research and Publication Ethics (RPE)** Course No.: **R-2**

Course Credits: **02**

Maximum Marks: **50**

Duration of Examination: **2 hrs**

Note: The candidates have to attempt five questions out of total ten, selecting at least one from each unit.

Course Title: Research and Publication Ethics (RPE)

Course Level: 2 Credit Course (30 hours)

Eligibility: M.Phil., Ph.D. students and interested faculty members (It will be made available to post graduate students at later date).

Fees: As per University Rules

Faculty: Interdisciplinary Studies

Qualifications of faculty members of the course:

Ph.D. in relevant subject areas having more than 10 years' of teaching experience.

Course Code: CPE-RPE

Course Structure:

The course comprises of five units listed in table below.

Unit No.	Unit Title	Teaching Hours
UNIT-1	Philosophy, Ethics and Scientific Conduct	8 hrs.
UNIT-2	Publication Ethics	7 hrs.
UNIT-3	Open Access Publishing	4 hrs.
UNIT-4	Publication Misconduct	4 hrs.
UNIT-5	Database and Research Metrics	7 hrs.

Unit-1: Philosophy, Ethics and Scientific Conduct

Introduction to philosophy: definition, nature and scope, concept, branches; Ethics: defining moral philosophy, nature of moral judgements and reactions; Ethics with respect to science and research, intellectual honesty and research integrity; Scientific misconducts: Falsification, fabrication and Plagiarism (FFP); Redundant publications: duplicate and overlapping publications, salami slicing; Selective reporting and misrepresentation of data.

Unit-2: Publication Ethics

Publication Ethics: definition, introduction and importance; Best practices/standards setting initiatives and guidelines: COPE, WAME, etc.; Conflicts of interest; Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa,

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types; Violation of publication ethics, authorship and contributorship; Identification of publication misconduct, complaints and appeals; Predatory publishers and journals.

Unit-3: Open Access Publishing

Open access publications and initiatives; SHARPA/RoMEO online to check publisher copyright & self-archiving policies; Software tool to identify predatory publications developed by SPPU; Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

Unit-4: Publication Misconduct

Group Discussions

Subject specific ethical issues, FFP, authorship; Conflicts of interest; Complaints and appeals: examples and fraud from India and abroad.

Software tools

Use of plagiarism software like Turnitik, Urkund and other open source software tools.

Unit-5: Database and Research Metrics

Databases

Indexing databases; Citation databases: Web of Science, Scopus, etc.

Research Metrics

Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics: h-index, g-index, i10 index, altmetrics.

REFERENCES:

Bird, A. (2006). Philosophy of Science, Routledge.

MacIntyre, Alasdair (1967) A Short History of Ethics: London.

P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN: 978-9387480865.

National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). On Being a Scientist: A Guide of Responsible Conduct in Research: Third Edition. National Academic Press.

Rensik, D.B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from <https://www.niehs.nih.gov/research/resources/bioethics/whatis>

Beall, J. (2012) Predatory publishers are corrupting open access. Nature, 489(7415), 179-179, <https://doi.org/10.1038/489179a>

Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019), ISBN: 978-81-939482-1-7. http://www.insaindia.res.in/pdf/Ethics_Book.pdf

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Course Title: **MOFs/CPs and Nanomaterials**

Course No.: **R-4(I)**

Course Credits: **06**

Maximum Marks: **150**

Duration of Examination: **3 hrs**

Note: The candidates have to attempt five questions out of total nine, selecting at least one from each unit.

- 1. Coordination Polymers (CPs) & Metal organic Frameworks (MOFs)**
Synthesis of Metal-Organic Frameworks (MOFs): Routes to Various MOF Topologies, Morphologies, and Composites:
Introduction, Historical Developments, MOFs vs Coordinations Polymers-general account, classifications of MOF/CPs on basis of dimensionality (1D, 2D and 3D), Covalent organic frameworks (COPs), porous organic polymers and related organic porous materials-general account.
Conventional Synthesis and Alternative Synthesis Routes: Microwave-Assisted Synthesis , Various Aspects of MOF Synthesis: Solvents and Structure-Directing Agents, a brief account on importance of temperature and autogenous pressure requirement in hydrothermal synthesis.
- 2. The Concept of Mixed Organic Ligands in Metal-Organic Frameworks:** Types of different ligands (hetero-atom(s) containing polycarboxylates) and their different bonding modes, Nodal auxiliary spacers and rigid pillared linkers in MOFs; 2D, 3D Pillared-layer mixed ligands MOFs and Rod shaped spacer mixed ligands, different topologies in MOF/CPs, Secondary building units (SBUs) a general account
Molecules encapsulation in MOFs and its applications—molecular gas cylinders (hydrogen, methane, acetylene), Sensing, adsorption and gas storage applications by Organic-Inorganic hybrid materials; H₂ /CO₂ gas storage and drug delivery
- 3. (a) Photo-Luminescent properties of MOF/CPs**
Luminescent metal–organic frameworks and coordination polymers as alternative phosphors for energy efficient lighting device
Introduction, Principle, Luminescence mechanisms in LMOF/LCP phosphors: Up-conversion & Down conversion, Rare earth metal based LMOFs/LCPs, Lanthanide LMOFs/LCPs with colored emission and Lanthanide LMOFs/LCPs with white emission.
(b) Catalytic properties of MOFs/CPs
Designing Metal-Organic Frameworks for Catalytic Applications: Introduction, Metal-Organic Frameworks as Catalysts
- 4. (a) Magnetic properties of MOF/CPs**
Brief review of different types of magnetic behaviours, spin-orbit coupling, quenching of orbital angular momenta, measurement of magnetic susceptibility and Magnetic momenta using VSM and SQUID methods, AC and DC magnetism- Field cooling (FC) and Zero field cooling (ZFC) a brief overview, Single molecular magnets (SMM) based on Dy MOFs and Applications of Lanthanide MOFs in MRI (Gd-MOFs).

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5. **Nano- Materials**

Background to Nanoscience: Definition of Nano, emergence and challenges of Nanoscience and nanotechnology, influence of nano over micro/macro, size effects and crystals, large surface to volume ratio, surface effects on the properties.

Types of nanostructure and properties of nanomaterials: One dimensional, Two dimensional and Three dimensional nanostructured materials (carbon age-new form of carbon: CNT to Graphene), Graphene and its Functionalization, Graphene Oxide, Carbon nanotubes (CNT) and their properties and applications. Core-Shell chemistry in nanomaterials & its significance. Mechanical, physical and chemical properties of nanomaterials

REFERENCES:

1. Inorganic Chemistry: Principles Of Structure And Reactivity, 4Th Edn. 2006. by Huheey, James E. & Keiter, Ellan E.
2. Coordination Polymers-Design, analysis & applications by Turner Neville Batten, RSC Publishing, ISBN: 9780854048373, 0854048375.
3. Main Group Metal Coordination Polymers: Structures and Nanostructures (English, Hardcover, Ali Morsali, Lida Hashemi).
4. W. Gaddand, D. Brenner, S.Lysherski and G.J.Infrate (Eds), Handbook of nanoscience, Engg and Technology, CRC Press,2002.
5. G.Cao, Naostructures and Nanomaterials: Synthesis, properties and applications, Imperical College Press, 2004.
6. J.George, Preparation of thin films, Marcel Dekker, InC., New York, 2005. 4. C.N.R.Rao, A.Muller, A.K.Cheetham (Eds), The chemistry of nanomaterials: Synthesis, properties and applications, Wiley VCH Verlag Gmbh&Co, Weinheim, 2004.
7. Intoduction to Nanotechnology- Charles P Poole & Frank J. Ownes.
8. Physical properties of Carbon Nanotube-R Satio.
9. Carbon Nanotubes: Properties and Applications- Michael J. O'Connell.
10. Nanotubes and Nanowires- CNR Rao and A Govindaraj RCS Publishing.
11. Nanoscale materials -Liz Marzan and Kamat 6. Carbon Nanomaterials for Environmental and Biological Applications, Bergmann and Machado., Springer.
12. "Introduction to Magnetic Materials" by B D Cullity.
13. "Magnetism and Magnetic Materials" by J P Jakubovics.
14. Photoluminescence Spectroscopy by James E. Toney.
15. Recent Reviews on studies on Coordination polymers and nanomaterials.

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Course Title: **Solid State Chemistry**

Course No.: **R-5(P)**

Course Credits: **06**

Maximum Marks: **150**

Duration of Examination: **3 hrs**

Note: The candidates have to attempt five questions out of total nine, selecting at least one from each unit.

Elementary idea of different type of metal oxides

Spinel ferrites, Inverse spinel ferrites, Mixed spinel ferrites, Perovskite oxides, Ruddlesden-Popper oxides, Pyrochlores, Their structures

Preparative strategies for bulk and nanomaterials

Different principles and reactions involved in methods of preparation of solid state materials: Ceramic method, Precursor method, Sol-gel method, Combustion methods

Characterization Techniques

X-ray diffraction, Indexing of planes, Evaluation of cell parameters from XRD data, Determination of crystallite size from XRD data,

Elementary idea of EDX, SEM and TEM, Explanation for surface morphology of some given SEM images in powder and pelletized form, Explanation for grain size and morphology of some TEM images of both nano and bulk forms of samples

Principle of X-ray photoelectron spectroscopy, Determination of oxidation state of elements in metal oxides

Methods of determination of oxygen stoichiometry in metal oxides using TGA and Iodometry methods

Magnetic Studies

VSM and Faraday methods for the determination of various magnetic parameters like saturation magnetization, Coercivity, Remanence, Magnetic susceptibility, Curie law, Curie-Weiss law

Transport properties

Determination of resistivity by PPMS and Four probe method, Various laws governing conduction mechanism in metal oxides like Arrhenius model, Polaron Hopping Model, Variable Range Hopping Model, Giant Magnetoresistance, Double-exchange and Super-exchange mechanisms

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Course Title: **Frontiers in Organic Chemistry** Course No.: **R-6(O)**

Course Credits: **06**

Maximum Marks: **150**

Duration of Examination: **3 hrs**

Note: The candidates have to attempt five questions out of total nine, selecting at least one from each unit.

Metal Catalyzed Reactions

Carbon-Carbon bond forming reactions (Suzuki, Heck, Sonogashira and Negishi coupling reactions).

Carbon-Nitrogen bond forming reactions (Buchwald-Hartwig reactions).

Carbon-Oxygen bond forming reactions.

Medicinal Chemistry

Strategies used in Analog design and SAR and QSAR.

Natural products as Leads for New Pharmaceuticals

Introduction, CNS systems, Anticancer (Taxol, Podophyllotoxin), Antiasthama (Ephedrine, Isoprenaline, Salbutamol).

Multicomponent reactions

Green aspects. Three & four component reactions for synthesis of heterocyclic compounds (Biginelli, Hantzsch, Passerini, Ugi and Bucherer-Berg's reactions, Robinson's synthesis of tropinone).

Name reactions and Reagents in organic synthesis

Larock Indole synthesis, Gabriel- Colman rearrangement, Eischenmoser reaction, Ramberg-Backlund olefin synthesis.

Methane sulfonic acid, DIBAL-H, Lithium diisopropylamide, Swern's reagent for oxidation, molecular oxygen (including activation with transition metals), 1,3-dithiane, MAD (Methyl aluminum bis(2,6-di t-butyl-4-methyl phenoxide)

Total Synthesis of natural products

Sparteine (Van Tamelen et al.), Pentalenene (G.Mehta et. al.), (±)- Retigeranic Acid (E.J. Corey et. al.), (+)-Pancratistatins (2017, David Sarlah et.al.).

BOOKS RECOMMENDED:

1. Multicomponent Reactions, J. Zhu, H. Bienayme, Wiley-VCH Verlag GmbH & Co. (2005).
2. Handbook of Green Chemistry, Prof. Paul T. Anastas, John Wiley & Sons.
3. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1: Principles and practice; Edited by Manfred E. Wolff, John Wiley and Sons (1995).
4. Multicomponent Reactions, J. Zhu, H. Bienayme, Wiley-VCH Verlag GmbH & Co. (2005).
5. Name Reactions and Reagents in Organic Synthesis, 2nd Edition, Bradford P. Mundy, Michael G. Ellerd, Frank G. Favalaro, Jr., Wiley (2005).

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Course Title: **Solution Chemistry**

Course No.: **R-7(P)**

Course Credits: **06**

Maximum Marks: **150**

Duration of Examination: **3 hrs**

Note: The candidates have to attempt five questions out of total nine, selecting at least one from each unit.

Solution Chemistry

Solute Solvent Interactions

The role of the solvent, energetic of solvation, the nature of solvent-solute interactions, measurement of solvent strength, effect of physical properties of the solvent, melting point and boiling point, heat of fusion and heat of vaporization, dielectric constant, viscosity, effect of chemical properties of the solvent, effect of acidic or basic characteristics of the solvent, chemical effects of solubility, effect of oxidizing and reducing characteristics, solvent characteristics of water type reactions in solvents, precipitation, salt formation, solvolysis, solvation.

Advanced Solution Thermodynamics

Ideal and non-ideal solutions, activity and activity coefficients, mixing and excess properties of liquid-liquid mixtures. Theories of solutions of electrolyte and non-electrolyte liquids, Van Laar theory, Van Der Waals theory, Scatchard-Hildebrand theory, Lattice theory, Prigogine Cell theory, Flory equation of state theory, Prigogine-Flory-Patterson theory, Extended Real Associated Solution model and Kirkwood-Buff theory.

Modern Experimental Techniques

Principle and working of DSA, Microviscometer, determination of vapour-liquid equilibrium by static and dynamic methods, heat capacity and heat of mixing by calorimeters, and determination of volumetric, transport, acoustic and optical properties of liquid-liquid mixtures. Thermodynamic relations of excess Gibbs energy, excess entropy, excess enthalpy, excess volume, viscosity deviation, excess heat capacity and excess compressibility. Partial molar properties, their physical significance and methods of their determination. Study of non-ideal behaviour of various types of solutions: nonpolar + nonpolar, polar + nonpolar, polar + polar, and mixtures hydrogen-bond formation and charge transfer complexes; interpretation in terms of molecular interactions.

BOOKS RECOMMENDED:

1. Prausnitz J.M., Lichtenthaler R.N., Azevedo E.G., Molecular Thermodynamic of Fluid-Phase Equilibria, (Prentice Hall, 3rd edition, 1998).
2. Rowlinson J.S., Liquid and Liquid Mixtures (Springer; 1st edition, 1995).
3. Acree W.E., Thermodynamic Properties of Nonelectrolyte Solutions (Academic Press, 1984).
4. J. Bevan Ott, Juliana Boerio-Goates, Chemical Thermodynamics: Advanced Applications (Academic Press, 1st edition, 2000).

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5. I. Prigogine, The Molecular Theory of Solutions (North Holland Publishing Co., Amsterdam, 1957).
6. Arie Ben-Naim, Molecular Theory of Solutions (Oxford University Press, USA, 2006).