

HIMACHAL PRADESH UNIVERSITY, SHIMLA-171005

FACULTY OF PHYSICAL SCIENCES



REVISED SYLLABI

FOR Ph.D. CHEMISTRY COURSE WORK

(Effective from Session 2024-25, beginning from the batch admitted in November, 2024 & onwards)

**DEPARTMENT OF CHEMISTRY
HIMACHAL PRADESH UNIVERSITY
SUMMER HILL, SHIMLA-171005, INDIA**

A Detailed Scheme and Course Contents of the Syllabi for Ph.D. Chemistry Course work
(Effective from Session 2024-25, beginning from the batch admitted in November, 2024 & onwards)

Each candidate has to study three courses in Ph.D Chemistry Course work.
Course I (Research and Publication Ethics), compulsory
Course II (Research Methodology), compulsory
Course III (only one course to be chosen out of three courses as per respective specialization i.e. Inorganic Chemistry, OR Organic Chemistry OR Physical Chemistry).

| Course | Course Code | Title of course | Max. Marks | Credit | Hours |
|--|----------------|--|------------|--------|-------|
| Course-I | RPE-PhD | Research and Publication Ethics (Common for all HPU Ph.D. programmes) | 50 | 2 | 30 |
| Discipline-wise course | | | | | |
| Course-II | CHE-RM-PhD-101 | Research Methodology (Compulsory for all Ph.D. Chemistry specializations) | 100 | 5 | 75 |
| Discipline-specific research oriented Elective course, only one course to be chosen as per specialization | | | | | |
| | | <u>INORGANIC CHEMISTRY</u> | | | |
| Course-III | CHE-PhD-102A | Advanced Inorganic Chemistry | 100 | 5 | 75 |
| | | <u>ORGANIC CHEMISTRY</u> | | | |
| | CHE-PhD-102B | Advanced Organic chemistry | 100 | 5 | 75 |
| | | <u>PHYSICAL CHEMISTRY</u> | | | |
| | CHE-PhD-102C | Advanced Physical Chemistry | 100 | 5 | 75 |

Note: The passing marks for Ph.D. course work will be 55% aggregate with minimum 50% in each individual course (all three courses).

Research and Publication Ethics
Course Code: RPE-PhD
(Common for all Ph.D. students)

Credit weightage: 2
Max. Marks: 50

Time allowed: 3 hours

Course description

This course has a total of 6 units focusing on the basics of philosophy of science and ethics, research integrity, and publication ethics. Hands-on sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open-access publications, research metrics (citations, h-index, Impact Factor, etc.), and plagiarism tools will be discussed in this course.

Objectives

- a. Promote the importance of research integrity.
- b. Discuss the principles of publication ethics.
- c. Educate on identifying research misconduct and predatory publishing.
- d. Discuss indexing and citation databases.
- e. Provide information on open-access publications and research metrics.
- f. Introduce various plagiarism detection tools.

Evaluation

Continuous assessment will be conducted through tutorials, assignments, quizzes, and group discussions. At the end of the course, a final written examination of 50 Marks will be conducted.

1. Students who have at least 75% attendance in classes will be considered eligible for the final written examination.
2. The exam will be conducted for a three-hour duration.

Note: The passing marks for Ph.D course work will be 55% aggregate with minimum 50% in each individual course (All three courses).

Note for Paper Setting

There will be 7 questions covering all the units. The first six questions (1, 2, 3, 4, 5 & 6) of 6 marks each will consist of one question from each unit, with internal choice provided, meaning there will be two questions from each unit. The 7th question will consist of 10 short answer type questions using Roman numerals (i, ii, iii,... x) each with 2 marks. There will be at least one question from each unit, and students will be required to attempt any seven questions out of ten.

Course contents: Research and Publication Ethics

Unit 01: Philosophy and Ethics

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgments and reactions

Unit 02: Scientific Conduct

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

Unit 03: Publication Ethics

1. Publication ethics: definition, introduction, and importance
2. Best practices/standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

Unit 04: Open Access Publishing

1. Open-access publications and initiatives
2. SHERPA/ROMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal, etc.

Unit 05: Publication Misconduct

A. Group Discussions

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

B. Software tools

Use of plagiarism software like Turnitin, Urkund, and other open-source software tools

Unit 06: Databases and Research Metrics

A. Databases

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics

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

Suggested Readings

- Beall, J. (2012). Predatory publishers are corrupting open access. *Nature*, Vol. 489(7415), 179.
<https://doi.org/10.1038/489179a>.
- Bird, A. (2006). *Philosophy of Science*. Routledge.
- Bretag, Tracey (2016). *The Handbook of Academic Integrity*. Springer.
- Chaddah, P. (2018). *Ethics in Competitive Research: Do not get scooped; do not get Plagiarized*. ISBN:978-9387480865.
- Grudniewicz, Agnes, D. Moher, Kelly D. Cobey+32 authors (2019). Predatory journals: no definition, no defense. *Nature*, Vol. 576.
- Indian National Science Academy (2019). *Ethics in Science Education, Research and Governance* (2019). ISBN:978-81-939482-1-7.
http://www.insaindia.res.in/pdf/Ethics_Book.pdf
- Israel, Mark, Iain Hay (2006). *Research Ethics for Social Scientists*. London.
- Lang, James M. (2013). *Cheating Lessons: Learning from Academic Dishonesty*. Harvard University Press.
- MacIntyre, Alasdair (1967). *A Short History of Ethics*. London.
- National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). *On Being a Scientist: A Guide to Responsible Conduct in Research*. Third Edition. National Academies Press.
- Resnik, D. B. (2011). *What is ethics in research & why is it important*. National Institute of Environmental Health Sciences, 1-10.
<https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm>
- Whitley Jr., Bernard E. & Patricia Keith-Spiegel (2001). *Academic Dishonesty: An Educator's Guide*. Psychology Press.

Course-II
Research Methodology
CHE-RM-PhD-101

Teaching Hours: 75
Credits: 5

Note for Paper Setting:

Time allowed: 3 hours
Max. Marks: 100

There will be 11 questions covering all the units.

The first 10 questions of explanatory answers (1,2,3,.....10) of 12 marks each and will consist of two questions from each unit (with internal choice provided). The students will be required to attempt one question from each unit.

The 11th question will be compulsory and will consist of 10 short answer type questions (using Roman numerals i,ii,iii,.....x) of 5 marks each, covering all the units. The students will be required to attempt any eight questions out of these ten questions.

The students can opt for MOOCs/SWAYAM and other accredited online platforms, with prior approval of relevant bodies.

Students with at least 75% attendance will be eligible for the final written examination.

Note: The passing marks for Ph.D. course work will be 55% aggregate with minimum 50% in each individual course (all three courses).

Course Description: This course has a total of 5 units focusing on the basics of research methodology, such as pure and applied research, exploring or formulative research, descriptive research, diagnostic research, scientific writing, writing of research paper, short communications, review articles, monographs, technical and survey reports, authored books, and edited books and dissertation concept of chemical safety, sustainable practices in chemistry, and applications of computer tools in research.

Course Objectives:

- Detailed discussion on various types of research methodologies.
 - Discussion on various scientific documents and their writing.
 - Educate students about important aspects of chemical safety.
 - Discuss sustainable practices in chemistry.
 - Provide information on computer applications in research.
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Course contents: Research Methodology

UNIT-I

Research Methodology: Types and methods of research, classification of research, pure and applied research, exploring or formulative research, descriptive research, diagnostic research/study, evaluation of research/study, action research, and experimental research-problem selection. Meaning, Scope, Primary sources of literature survey, Journals, patents etc., secondary sources of literature survey, Books, Reference books, Text books, listing of letters.

UNIT-II

Scientific Writing: Scientific Document; Organization and writing of research paper, short communications, review articles, monographs, technical and survey reports, authored books, and edited books and dissertation. Abstracts and Journals in chemistry, Electronic forms of Journals, major libraries, subscribing Journals related to chemistry in the region and country and Patents and Patents writing.

UNIT-III

Concepts of Chemical Safety: Chemical safety and ethical handling of chemicals, safe working procedure and protective environment, emergency procedure and first aid, laboratory ventilation, safe storage and use of hazardous chemicals.

UNIT-IV

Sustainable Practices in Chemistry: Procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmosphere, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, principles of green chemistry (with one example of each principle).

UNIT-V

Computer Applications in Research: Application and uses of common softwares in chemistry-origin, chemsketch, chemdraw, basic ideas on the use of internet in chemistry education.

Reference Books:

- 1 William Kemp, Organic Spectroscopy, ELBS London, 1987.
- 2 RM Silverstein, CG Bassler and TC Morrill, Spectroscopic Identification of Organic Compounds, 4th Edition, John Wiley & Sons, New York, 1981.
- 3 Donald L Pavia, Gary M Lampman and George S Kriz, Introduction to Spectroscopy, 3rd Edition, Saunders Golden Sunburst Series.
- 4 CN Banwell and Elaine M McCash, Fundamentals of Molecular Spectroscopy, 4th Edition.
- 5 Raymond Chang, Basic Principles of Spectroscopy, RE Krieger Publishing Co., Huntington, New York, 1978.
- 6 Paul D Leedy, Jeanne E Ormrod and Jeanne Ellis Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.
- 7 Robert V Smith, Graduate Research: A Guide for Students in the Sciences, University of Washington Press, 1998.
- 8 Anthony M Graziano and Michael L Rau, Research Methods: A Process of Inquiry, Prentice Hall, 2006.
- 9 Peter C Jurs, Computer Software Applications in Chemistry, 2nd Ed., John Wiley & Sons, New York, 1996.
- 10 Practical Skills in Chemistry, J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd. [Prentice Hall] (2002)
11. Research Methodology. Methods and Techniques : C. R. Kothari,

Course-III
Advanced Inorganic Chemistry
CHE-PhD-102A

Teaching Hours: 75
Credits: 5

Note for Paper Setting:

Time allowed: 3 hours
Max. Marks: 100

There will be 11 questions covering all the units.

The first 10 questions of explanatory answers (1,2,3,.....10) of 12 marks each and will consist of two questions from each unit (with internal choice provided). The students will be required to attempt one question from each unit.

The 11th question will be compulsory and will consist of 10 short answer type questions (using Roman numerals i,ii,iii,.....x) of 5 marks each, covering all the units. The students will be required to attempt any eight questions out of these ten questions.

The students can opt for MOOCs/SWAYAM and other accredited online platforms, with prior approval of relevant bodies.

Students with at least 75% attendance will be eligible for the final written examination.

Note: The passing marks for Ph.D. course work will be 55% aggregate with minimum 50% in each individual course (All three courses).

Course Description:

This course has a total of 5 units focusing on the basics of Advanced Inorganic Chemistry. The course focuses on providing students the understanding of advanced topics of Inorganic Chemistry such as reactions at coordinated ligands, electron-transfer reactions of complexes, catalysis involving organometallic compounds, catalysis involving organometallic compounds, voltammetric methods of analysis, supramolecular reactions and catalysis.

Objectives:

- To provide the knowledge and understanding of reactions at coordinated ligands and electron transfer reactions of metal ligand complexes.
- To impart knowledge about synthesis of new metal complexes leading to the development of advanced inorganic chemistry.
- To provide knowledge in the field of catalysis involved in organometallic chemistry and polymerization extensively useful in research and industry.
- To develop analytical skills, experimental skills and critical thinking of students and equip them to collect, interpret data and apply it different fields to resolve complex chemical problems.
- To impart specific knowledge about Supramolecular chemistry including reactions and catalysis and supramolecular assemblies and their applications

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Course contents: Advanced Inorganic Chemistry

UNIT-I

Reactions at Coordinated Ligands:- Reactions due to metal ion polarization of co-ordinated ligands, Aldol Condensation, Imine formation, hydrolysis and substituent exchange. Template effect and macrocyclic ligands.

Electron-Transfer Reactions of Complexes: Electron-transfer theory, Outer-sphere exchange reaction. Bridge mechanism, Two-electron transfers, Non-complementary reactions. Replacement through Redox Mechanism, Photochemical Reactions of Chromium and Ruthenium complexes.

UNIT-II

Synthesis of Coordination compounds:- Theoretical consideration: Labile and Inert Coordination compounds, synthesis of mixed ligand complexes by co-propotionation, chelate effect, trans effect (Peyrone's rule, Jorgonson's rule and Kurnakov's rule), Cis effect, Geometric isomerization of square planer platinum(II) and Palladium(II) complexes, hard-soft acid-base (HSAB) principle, factors affecting the acid base properties of coordination compounds, ligand effects on redox potentials of coordination compounds.

UNIT-III

Catalysis Involving Organometallic compounds: Homogeneous hydrogenation and hydroformylation of unsaturated compounds (Olefins). Hydroformylation, hydrosilylation of unsaturated compounds, hydrocyanation of alkenes; alkenes and alkynes metathesis.

Co-ordination Addition Polymerisation: Zeigler Natta catalysts, composition, nature and mechanism of stereo specific placement in polymerisation, bimetallic and monometallic mechanism, stereoregulation, Supported metal oxide catalysts, polymerisation mechanism, bound-ion radical mechanism and bound-ion co-ordination mechanism. Metallocene based Zeigler Natta catalysts, catalysts composition, active centre and polymerisation mechanism.

UNIT-IV

Voltammetric methods of analysis: Principle, excitation signals, mass transfer mechanism, instrumentation, methods of analysis and applications of pulse polarography, cyclic voltammetry and anode stripping voltammetry. Use of cyclic voltammetry for the determination of formal reduction potential and number of electron change for ferri/ferrocyanide couple and to study electrode mechanisms of electron reduction of nitrobenzene and voltammetry with microelectrodes.

UNIT-V

Supramolecular Reactions and Catalysis: Introduction, Catalysis by reactive macrocyclic cation receptor molecule, by reactive macrocyclic anion receptor molecule, Supramolecular metallocatalysis.

Supramolecular Assemblies: Introduction, Supramolecular solid materials, Molecular recognition at surfaces (Endoreceptors vs Exoreceptors), Molecular and Supramolecular Devices, Photonic, electronic and Ionic Devices.

Books Recommended:

1. Homogeneous transition metal catalysis – Christopher Masters
2. Principles and Application of Homogeneous Catalysis – Nakamura and Tsutsui
3. Advanced Polymer Chemistry- Manas Chanda
4. Synthetic Coordination Chemistry: Principles and Practice- J.A. Davies, C.M. Hockensmith, V.Y.Kukushkin and Y.N. Kukushkin.
5. Fundamentals of Analytical Chemistry- Skoog, West, Holler and Crouch
6. Chemistry experiments for Instrumental methods- Sawyer, Heineman and Beebe.
7. Electronic absorption spectroscopy and related techniques: D.N. Sathyanaray.
8. The Organometallic Chemistry of Transition metals: R.H. Crabtree.
9. Principles and applications of organotransition metal chemistry by Collman and Hegden
10. Elements of Bioinorganic Chemistry- G.N. Mukherjee and Arabinda Das (1993).
11. Inorganic Chemistry - Purcell and Kotz.
12. The Inorganic Chemistry of Biological Process-M.N. Hughes (2nd Edn.)
13. Inorganic Reaction Mechanism- Edward.
14. Inorganic Reaction Mechanism - Bassolo and Pearson.
15. Supramolecular Chemistry concepts and Perspectives- Jean-Marie Lehn(VCH-1995)

Course-III
Advanced Organic chemistry
CHE-PhD-102B

Teaching Hours: 75
Credits: 5

Note for Paper Setting:

Time allowed: 3 hours
Max. Marks: 100

There will be 11 questions covering all the units.

The first 10 questions of explanatory answers (1,2,3,.....10) of 12 marks each and will consist of two questions from each unit (with internal choice provided). The students will be required to attempt one question from each unit.

The 11th question will be compulsory and will consist of 10 short answer type questions (using Roman numerals i,ii,iii,.....x) of 5 marks each, covering all the units. The students will be required to attempt any eight questions out of these ten questions.

The students can opt for MOOCs/SWAYAM and other accredited online platforms, with prior approval of relevant bodies.

Students with at least 75% attendance will be eligible for the final written examination.

Note: The passing marks for Ph.D course work will be 55% aggregate with minimum 50% in each individual course (All three courses).

Course Description: This course has a total of 5 units focusing on the basics of Advanced Organic Chemistry. The course focuses primarily on providing students the understanding of advanced topics of Organic Chemistry such as various spectroscopic techniques, such as UV, IR, NMR and mass spectrometry in organic compounds and solving problems based on these techniques, mechanisms of various organic reactions, techniques of polymer synthesis, special polymer reactions including copolymer synthesis and drug design and development.

Course Objectives:

- To provide the students advanced knowledge about the principles and instrumentation of spectroscopic techniques, such as UV, IR, NMR and mass spectrometry in organic compounds.
- To understand mechanistic details of different types of rearrangement reactions, use of a few reagents used in organic synthesis.
- To understand the fundamental concepts of polymerization, to know about various types of polymerization reaction and their mechanisms.
- To learn the various techniques of polymer and copolymer synthesis.
- To impart advance knowledge of medicinal chemistry and the procedures of various drug design strategies.

Course contents: Advanced Organic chemistry

UNIT –I

Spectroscopy: Basic theory, Instrumentation and applications of UV spectroscopy, IR Spectroscopy, NMR Spectroscopy and Mass spectrometry in organic compounds. Problems based on IR, UV, NMR and mass spectral data.

UNIT - II

Reaction –Mechanism: Reaction and mechanism of following organic reactions: Stevens rearrangement, Cope rearrangement, Claisen rearrangement, Metathesis of olefins, Di- π methane rearrangement, Hofmann-Löffler reaction, Sharpless asymmetric epoxidation and Stork-enamine reaction.

Reagents in Organic Synthesis: Reagents in organic synthesis: Wilkinson catalyst, Triphenylphosphine-alkyl halide reagent, Lithium dialkyl cuprates (Gilman's reagents), Lithium diisopropylamide (LDA), Dicyclohexylcarbodiimide (DCC), and Tri-n-butyltinhydride. Nickel tetracarbonyl, Trimethylchlorosilane.

UNIT–III

Polymer Synthesis: Kinetics and mechanism of radical, cationic, and anionic addition polymerization, Living polymerization. Significance of chain transfer reactions, Chemistry and kinetics of inhibition and retardation.

Miscellaneous polymerization reactions: Monomers with two different polymerizable groups, Hydrogen transfer polymerization, Polymerization and cyclotrimerization of isocyanates, Monomers with triple bonds, *Ring opening polymerization:* polymerization mechanism and kinetics, examples of cyclic amide and ethers.

Copolymer Synthesis: Principles of polymer reactivity, factors affecting polymer reactivity, Chain transfer copolymerization, Chemistry and methods of graft copolymerization, radical graft copolymerization, ionizing and UV radiation and redox initiation, and other grafting systems. Block copolymer formation, sequential monomer addition.

UNIT- IV

Special Polymer Reactions: General introduction to the polymer reactions, derivatization reactions of biopolymers – cellulose, and starch. Polymer as carriers or supports, polymeric reagents, polymeric substrates, polymeric catalysts,

Specialty Polymers: Biodegradable polymers (lactic and glycolic acid based). Conducting polymers, applications of conducting polymers. Hydrogels and their applications. Biomedical polymers, contact lenses, dentures and implants. Problems of non-degradability of synthetic polymers, biomass utilization.

UNIT- V

Drug design and development: Pharmacokinetics and Pharmacodynamics: Introduction to drug absorption, distribution, metabolism, elimination using pharmacokinetics. Importance of pharmacokinetics in drug development. Drug design, concepts of lead compound and lead modification, Example: Development of cimetidine-A rational approach to drug design: Anti-ulcer therapy, Biological activity of cimetidine ,Structure and activity of cimetidine, Metabolism of cimetidine, cimetidine analogues.

Books Recommended:

1. Practical NMR Spectroscopy, M.L.Martin, J.J. delpeuch and G.J.Martin, Heyden.
2. Spectrophotometric Identification of Organic Compounds, R.M. Silverstein, G.C.Bassler and T.C.Morrill, John Wiley.
3. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fischer and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry, D.H.Williams, I.Fleming, Tata McGraw-Hill.
6. Organic Spectroscopy by Jagmohan.
7. Organic Spectroscopy by W. Kemp.
8. Organic Synthesis: Jagmohan Singh and Yadav
9. Organic Synthesis: Feiser and Feiser.
10. An Introduction to Medicinal Chemistry, Graham L. Patrick.
11. Medicinal Chemistry: Principles and Practice Edited by F.D. King.
12. Textbook of Organic Medicinal and Pharmaceutical Chemistry, Edited by Charles O. Wilson, et al.
13. Introduction to Medicinal Chemistry, Alex Gringuage.
14. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
15. Polymer Science, V.R. Gowarikar, N.V. Visvanathan and J. Sreedhar, Wiley Eastern.
16. Functional Monomers & Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
17. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
18. Physics & Chemistry of Polymers, J.M.G. Cowie, Blakie Academic and Professional.
19. Polymer Chemistry and Physics of Modern Materials, J.M.G. Cowie and V. Arrighi,Taylor and Francis Group 2008.
20. Designing Safer Polymers by P.T.Anastas, P.H. Bickart, M.M. Kirchhoff , Wiley Interscience, 2001.

Course-III
Advanced Physical chemistry
CHE-PhD-102C

Teaching Hours: 75
Credits: 5

Note for Paper Setting:

Time allowed: 3 hours
Max. Marks: 100

There will be 11 questions covering all the units.

The first 10 questions of explanatory answers (1,2,3,.....10) of 12 marks each and will consist of two questions from each unit (with internal choice provided). The students will be required to attempt one question from each unit.

The 11th question will be compulsory and will consist of 10 short answer type questions (using Roman numerals i,ii,iii,.....x) of 5 marks each, covering all the units. The students will be required to attempt any eight questions out of these ten questions.

The students can opt for MOOCs/SWAYAM and other accredited online platforms, with prior approval of relevant bodies.

Students with at least 75% attendance will be eligible for the final written examination.

Note: The passing marks for Ph.D course work will be 55% aggregate with minimum 50% in each individual course (All three courses).

Course Objectives:

- To understand thermodynamics and molecular interactions in liquid mixtures.
- To explore the fundamentals of electrochemistry and electrode kinetics.
- To acquire knowledge of electrochemical methods.
- To understand and explore the spectroscopic methods.
- To investigate unique properties, synthesis and applications of nanomaterials.

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Course contents: Advanced Physical Chemistry

Unit-I

Thermodynamics and Molecular interactions in liquid mixtures: Ion-ion interactions, Ion-dipole interactions, Dipole-dipole interactions, Ion-induced dipole interactions, Dipole induced dipole interactions, Quadruple-octuple interactions; specific interactions, hydrogen bonding, charge-transfer interactions and contact charge-transfer interaction. Masson's equation, Jones-Dole equation and Kraus-Bray conductivity equation. Thermodynamic of excess functions; excess molar volumes, excess molar enthalpies, excess isentropic compressibility, excess Gibbs free energy, excess heat capacity and their significance. Statistical theories of liquid mixtures; (i) Cell model (ii) Flory's theory (iii) Sanchez and Lacombe's theory, Techniques for measuring speed of sound by DSA and Interferometer.

Unit-II

Electrodictics: Electron transfer under an interfacial electrical field, Butler-Volmer equation; electrode kinetic involving semiconductor solution interface, photo- electrochemistry; p-type photo-cathodes, n-type photo-anodes; Rate determining step in photo-electrochemical reaction, Ionic conductivity in solids; Solid electrolytes, Fast-ion conductors, oxygen ion conductors, sodium ion conductors, Solid state ionic devices, Batteries: Battery Performance Factors, Lithium batteries, Sodium batteries, fuel cells, supercapacitors.

Unit-III

Electrochemical methods: Cyclic Voltammetry: Principles and applications of cyclic voltammetry, Ilkovic equation, Randle-Sevcik equation, principle of coulometry at controlled potential and at constant current and its applications, Galvanostatic Charge-Discharge (GCD), Electrochemical Impedance Spectroscopy (EIS).

Unit IV

Spectroscopic Methods: Principle, instrumentations and applications of UV-Visible, FTIR, XRD, Fluorescence, NMR, XPS, SEM, TEM, AFM, TGA, particle size analyser, Mass spectroscopy, Raman spectroscopy and BET.

Unit V

Nanomaterials: Microstructure and defects in monocrystalline Materials-Effect of Nano dimensions on material behaviour Optical Properties, Electrical Properties, Mechanical Properties, Magnetic Properties

Synthesis Routes: Bottom-Up approaches – Top-Down approaches- Consolidation of Nano powders Mechanical Grinding, Wet Chemical Synthesis of Nanomaterials –Sol Gel Process, Gas Phase Synthesis, Flame assisted ultrasonic spray pyrolysis, Gas Condensation Processing, Hydrothermal method, Chemical Vapour Condensation (CVC).

Applications: Nanoelectronics, Nano optics, Nanoscale Chemical Biosensing, Biological/Biomedical Applications, Photovoltaics- Fuel Cells, Batteries, And Energy Related Applications, Nano energetics.

Suggested Readings:

1. Textbook of Physical Chemistry V by B.R. Puri , L.R. Sharma , M.S. Pathania & Manpreet Kaur; Vishal Publications
2. Instrumentation methods of analysis, Chatwal & Anand, Himalaya Publications.
3. Principles of Analytical Chemistry by Vacarcel, Springer Publications.
4. R.S. Drago, Physical Methods for Chemistry, Saunders Company
5. Text Book of Nanoscience and Nanotechnology by B S Murty , P Shankar , Baldev Raj, B B Rath, James Murday – Springer and University Press.
6. Introduction to Nanomaterial - Alagarasi, A, -2016-Research Gate.
7. Modern Electrochemistry 2A, Fundamentals of Electrodics; John O'M. Bockris , Amulya K. N. Reddy , Maria Gamboa-Aldeco
8. Modern Electrochemistry 2nd Edition Vol 1, Ionics; John O'M. Bockris , Amulya K. N. Reddy
9. Electrochemical Energy Storage: Batteries, Fuel Cells, and Hydrogen Technologies, 1st Edition by Slobodan Petrovic, Peter Kurzweil, Jürgen Garche, ISBN: 9781260012002, Publication Date & Copyright: 2022McGraw Hill.
10. Electrochemical methods: Fundamentals and applications 3E Hardcover – Import, 26 May 2022 by Allen J. Bard, Larry R. Faulkner, Henry S. White; Wiley
11. Methods in Physical Chemistry, Editor(s): Prof. Rolf Schäfer, Prof. Peter C. Schmidt, Print ISBN: 9783527327454 |, Online ISBN: 9783527636839 |DOI: 10.1002/9783527636839, Copyright © 2012 Wiley-VCH Verlag GmbH & Co. KGaA
12. Materials Characterization: Introduction to Microscopic and Spectroscopic Methods Yang Leng, ISBN-13: 978-0470822982 Publisher Wiley-Blackwell