

DRAFT *SYLLABUS FOR*
PH. D. COURSE WORK IN CHEMISTRY

Department of Chemistry
Kazi Nazrul University
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Kazi Nazrul University
Department of Chemistry
Draft Syllabus for Ph. D. Course Work in Chemistry
[with effect from the session 2017-2018]

Duration: 6 months

Total marks: 150

Paper	Topic	Full marks	Duration for class
Paper-I	Research design; Research Methodology; Tools and Methods Used in Chemical Research; Computational Aids; Dissemination	50 (4 credit)	30 L (30 h)
Paper-II	Instrumental methods and application in chemical analysis: use of different instruments like UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, NMR, Mass Spectrometer, SEM, HRTEM etc in various chemical analyses and computer simulation, X-ray Diffraction and Structural Analysis in Crystallography.	50 (4 credit)	30 L (30 h)
Paper-III	Ila: Optional-I	Term paper on Review of previous research works/ Literature Survey	50 Not less than 8000 words excluding references
	Iib: Optional-II	Chemistry in Nanoscience and Nanotechnology	50 30 L (30 h)
	Iic: Optional-III	Green Chemistry; Host-Guest Compounds; Crystal Engineering; Kinetic Aspects of Chemical and Biochemical Reactions	50 30 L (30 h)

Questions pattern

- (i) 10 marks will be allotted for internal assessments in each paper
- (ii) Total eight questions each with 8 marks to be set in each theoretical paper; examinees to be answered a total of five questions
- (ii) Duration of examination: 2 hrs for each theoretical paper of 50 marks
- (iii) For term paper/project work: internal assessment, 10; presentation of seminar in presence of external expert; 30, and thereafter interaction, 10

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[I L = 1.5 h]

Paper – I: Compulsory: 100 marks

1. Research design

6 L

Concept and model: theory building, testing and construction; descriptive and explanatory research; prediction, correlation and causation; deterministic and probabilistic views, pragmatization, social impact.

2. Research Methodology

8 L

Background; scope, aim and objectives; work elements and milestones; sampling; diagnostic tools; instrumentation - fabrication, interfacing; qualitative, quantitative and admixed methods; controlled trials for facile route(s); deterministic and probabilistic approaches; conjunctive study, parametric statistics; precision and confidence level; synergistic benefit of experiment and theory; connotation; outcome; discussion on research ethics

3. Tools and Methods Used in Chemical Research

5 L

Applicability of HPLC, GC, SFC, CE; microwave digester and reactor system; flow injection system; stopped flow spectrometer; SEM, TEM, AFM; transient absorption analyzer, fluorescence confocal microscope; diffractometer

4. Computational Aids

8 L

Handling of search engines like SciFinder, Cross Fire, CAS etc. for identifying and highlighting the research problem; treatise of the research data using softwares like STATISTICA, ORIGIN etc.; data analysis involving regression and curve fitting; calculation of chemical parameters using different modern scientific programs.

5. Dissemination

3 L

Layout; exchange of knowledge: demonstration; communication: oral and poster presentation in seminar/conference/symposium/workshop; posting in the web site; publication; break-through.

Suggested Readings

1. Research Methodology: Methods and Techniques, 2nd edn., C.R. Kothari, Wishwa Prakashan, New Delhi, 1990.
2. Denzin, Norman K. & Lincoln, Yvonna S. (Eds.). (2005). The Sage Handbook of Qualitative Research (3rd ed.). Thousand Oaks, CA: Sage. ISBN 0-7619-2757-3.

3. Loseke, Donileen R. & Cahil, Spencer E. (2007). "Publishing qualitative manuscripts: Lessons learned". In C. Seale, G. Gobo, J. F. Gubrium, & D. Silverman (Eds.), *Qualitative Research Practice: Concise Paperback Edition*, pp. 491-506. London: Sage. ISBN 978-1-7619-4776-9.
4. Marshall, Catherine & Rossman, Gretchen B. (1998). *Designing Qualitative Research*. Thousand Oaks, CA: Sage. ISBN 0-7619-1340-8.
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6. Guba, E. G., & Lincoln, Y. S. (2005). "Paradigmatic controversies, contradictions, and emerging influences" In N. K. Denzin & Y. S. Lincoln (Eds.), *The Sage Handbook of Qualitative Research* (3rd ed.), pp. 191-215. Thousand Oaks, CA: Sage. ISBN 0-7619-2757-3.
7. Denzin, Norman K. & Lincoln, Yvonna S. (2005). "Introduction: The discipline and practice of qualitative research". In N. K. Denzin & Y. S. Lincoln (Eds.), *The Sage Handbook of Qualitative Research* (3rd ed.), pp. 1-33. Thousand Oaks, CA: Sage. ISBN 0-7619-2757-3.
8. Adler, P. A. & Adler, P. (1987). *Membership roles in field research*. Newbury Park, CA: Sage. ISBN 978-0803927605.
9. Creswell, J. W. (2003). *Research design: Qualitative, quantitative, and mixed method approaches*. Thousand Oaks, CA: Sage Publications.
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12. Holliday, A. R. (2007). *Doing and Writing Qualitative Research*, 2nd Edition. London: Sage Publications.
13. Miles, M. B. & Huberman, A. M. (1994). *Qualitative Data Analysis*. Thousand Oaks, CA: Sage Publications.
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15. Taylor, Steven J., Bogdan, Robert, *Introduction to Qualitative Research Methods*, Wiley, 1998, ISBN 0-471-16868-8.
16. Wolcott, H. F. (1995). *The art of fieldwork*. Walnut Creek, CA: AltaMira Press.
17. Commonwealth of Learning, Module A5: *Mixed research methods*, Christine Spratt, Rob Walker and Bernadette Robinson, Terry Allsop, Richard Freeman and Bernadette Robinson, 2004, ISBN 1-894975-14-6.

18. N. K. Denzin, Y.S. Lincoln (eds.). Handbook of Qualitative Research. London: Sage Publications, 2000.
 19. Cohen J (1988). Statistical power analysis for the behavioral sciences (second edition). Hillsdale, New Jersey: Lawrence Erlbaum.
 20. Y.L. Lyubchenko, B.L. Jacobs, S.M. Lindsay, A. Stasiak, Atomic force microscopy of nucleoprotein complexes, Scanning Microsc. 1995, 9(3):705.
 21. Yuri L. Lyubchenko and Luda S. Shlyakhtenko, Visualization of supercoiled DNA with atomic force microscopy in situ, Proc Natl Acad Sci U S A. 1997 January 21; 94(2): 496–501.
 22. Franz J. Giessibl, Advances in atomic force microscopy, Reviews of Modern Physics, 2003, 75: 949.
 23. Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Pérez, S. Morita, O. Custance,). "Chemical identification of individual surface atoms by atomic force microscopy". Nature 2007, 446: 64.
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 25. R. V. Lapshin, Automatic drift elimination in probe microscope images based on techniques of counter-scanning and topography feature recognition, Measurement Science and Technology, 2007, 18 (3): 907.
 26. G. Schitter, M. J. Rost Scanning probe microscopy at video-rate" (PDF). Materials Today, 2008, 11: 40.
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Paper – II: Compulsory: 100 marks

Instrumental methods and application in chemical analysis: use of different instruments like UV-Vis, FTIR, Fluorimeter, Thermal Analyser, CHN(S) Analyser, NMR, Mass Spectrometer, SEM, HRTEM etc in various chemical analyses and computer simulation, X-ray Diffraction and Structural Analysis in Crystallography.

Paper-III: One optional paper from the followings: 100 marks

IIa: Optional-I

Term paper on Review of previous research works/Literature Survey

[Not less than 8000 words excluding references]

IIIb: Optional-II

1. Transformations and Rearrangements 10 L

Organic synthetic methodology, advances in organo-metallation and organic reagents in organic synthesis, stereo-selective conjugate additions, metal assisted/catalysed allylation, Heck reaction.

2. Advanced Spectroscopy and Hyphenated Systems 8 L

Advanced spectroscopic application in molecular structure analysis, ^{13}C -NMR, COSY, DOSY, NOESY, MALDI-TOF-MS, GC-MS, LC-MS, ICP-AES, ICP-MS.

3. Drug Design and Chemotherapy 10 L

Design and synthesis, pharmacokinetics, binding site, metabolism, administration, speciation, tolerance, regulation, potency, chiral drug, conformational restraint, eudismic ratio and Pfeier's rule, drug patenting; diagnostic and therapeutic agents in chemotherapy, strategic approaches, physiological binding to living organ/DNA, anticancer drugs of latest generation, trends and future challenges.

4. Bioactive Molecules 10 L

Preambles, biochemical self assembly, allosterism, preorganisation and complementarily, semiotics, biogenesis of carbohydrates, biosynthesis of aminoacids, fatty acids sterols, terpenoids, proteins, lipids, nucleic acid, heme & prostaglandins, transcription, enzymes, biocatalysis, DNA-RNA relationship, DNA-genome, glycomics etc..

IIIc: Optional-III

1. Spectroscopy and Dynamics of Excited States 8 L

Instrumentation, fluorescence (steady state and time-resolved) spectrometers, Time-dependent perturbation theory – Fermi's golden rule, LASER and non-linear interaction, femtosecond chemistry, Forster distance and cycle.

2. Quantum and Computational Chemistry 12 L

Multi-electron wave function, Hartree product and Hartee-Fock SCF wave function, HF-LCAO method, basis set, post HF methods and correlation energy, density functional theory(DFT), Thomas-Fermi model, Hohenberg-Kohn theorem and Kohn-Sham equations, Electronegativity and chemical potential, Fukui function in respect of reactivity; demonstration with Gaussian program.

3. Advanced Thermodynamics 6 L

Microscopic reversibility, Onsager reciprocity relation, Curie-Prigogine principle, Prigogine's theorem for stationary state, applications to chemical and biological process.

4. X-ray Diffraction and Structural Analysis in Crystallography 10 L

Fundamentals, HM notation, indexing of lattice planes, stereographic projection, Cu-K α and Mo-K α radiations, X-ray diffraction, Bragg refraction in terms of reciprocal lattices, Brillouin zones, crystal mounting, data collection, methods of analysis of single crystals structure, absorption correction structure solution and refinement, Z- value, R-value, GOF of data analysis, handling of soft wares like ORTEP, PLATONS, MERCURY, DIAMOND etc. for drawing the crystal structures using data files (.ins, .cif, .hkl files).

5. Chemistry in Nanoscience and Nanotechnology **8 L**

General concepts and consideration, synthetic strategies and characterization of different nano-materials using electronic microscopes like SEM, TEM, AFM etc., nano-tubes in hydrogen storage, nano-particles for medicinal purpose, current challenges and future trends.

IId: Optional-IV

1. Advanced Trace and Ultratrace Analysis **10 L**

Concepts and methodology, probes, variations, mechanistic study of chemical reactions, tracer packet, applications in research, industry, biology; interpretation of chemical and biochemical processes, acceleration mass spectrometry, genesis, engineering and production of radiopharmaceuticals for therapeutic and diagnostic purposes.

2. Green Chemistry **8 L**

Facets of green chemistry, green catalysts, synthesis and technology, the concept of zero discharge, applications of supercritical fluids and ionic liquids, eco-friendly biopolymers, biofuels, energy sources, laboratory experiments, alternative fluorocarbons and corrosion inhibitors, green chemistry and sustainable agriculture.

3. Host-Guest Compounds **10 L**

Non-covalent interaction, biological inspiration, inter-component bond, action and reaction, behavior of molecular individuals and populations, lock and key principle in molecular recognition, enantio-selective recognition chemical sensors, chemodosimeter, .molecular switches; natural and synthetic molecular receptors, application in chemical reactions, dendrimer chemistry and, biological assembly and disassembly.

4. Crystal Engineering **8 L**

Crystal-directed synthetic strategy, Kitaigorodskii's Aufbau principle, Fostering optoelectronics, non-linear optical activity, thermochromism, magnetism, catalysis, biomineralisation, biomimetics.

5. Kinetic Aspects of Chemical and Biochemical Reactions **8 L**

Handling of kinetic data, dimensional analysis of Eyring equation, exchange reactions and McKay plots, Marcus cross-correlation, reactions in organized assemblies and disassemblies in biological systems.

Suggested Readings*

1. G. C. Schatz and M. A. Ratner, Quantum mechanics in chemistry, Dover publications, Inc., New York, 2002.
2. D. A. McQuarrie, Quantum chemistry, Viva books Pvt. Ltd, New Delhi, 2003.
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20. B. Cornils, W. A. Harrman and R. Schlogl (Eds), *Catalysis from A to Z: A concise encyclopedia*, John Wiley & Sons, New York, 2000.
21. S. T. Langerwall, *Ferroelectric and antiferroelectric liquid crystals*, Wiley-VCH, Weinheim, 1999.
22. J. S. Miller and M. Drillon (Eds.), *Magnetism: from molecules to materials V*, Wiley-VCH, Weinheim, 2005.
23. M. Kohler and W. Fritzsche, *Nanotechnology: an introduction to nanostructuring techniques*, Wiley-VCH, Weinheim, 2004.
24. P. Ajayan, L. S. Schadler and P. V. Braun, *Nanocomposite science and technology*, Wiley-VCH, Weinheim, 2003.
25. B. Bhusan (Ed.), *Springer handbook of nanotechnology*, Springer, Berlin, 2004.
26. C. Doller (Ed.), *Therapeutic drugs*, 2nd edn, Churchill Livingstone, Edinburgh, 1999.
27. R. Silverman, *The organic chemistry of drug design and drug action*, Academic Press, New York, 1992.
28. D. Lednicer, *The organic chemistry of drug synthesis*, vol. 6, Wiley, New York, 1998.
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30. G. Patrick, *Medicinal chemistry*, Viva Books Pvt. Ltd., New Delhi, 2000.
31. F. D. King (Ed.), *Medicinal chemistry: principles and practice*, 2nd edn, Royal Society of Chemistry, 2002.
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33. T. A. Brown, *Genomes*, BIOS Scientific Publishers Ltd., Oxford, 1999.
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47. G. Rothenberg, Catalysis: Concepts and green applications, Wiley-VCH, Weinheim, 2008.
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57. C. A. Schalley (Ed.), Analytical methods in supramolecular chemistry, Wiley-VCH, Weinheim, 2007.
58. R. A. van Santen and M. Neurock, Molecular heterogeneous catalysis, Wiley-VCH, Weinheim, 2006.
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62. C. Hammond, The basis of crystallography and diffraction, Oxford University Press, New York, 2001.

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 65. G. G. Hammes, *Thermodynamics and kinetics for the biological sciences*, Wiley, Hoboken, New Jersey, 2000.
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*In addition to the above mentioned references, the Journals of ACS, RSC, Elseviers, Springer, Taylor & Francis etc. publishers should also be consulted