

University of Pune

Department of Chemistry

Syllabus for M.Phil. / Ph.D. course in Chemistry
(to be implemented from academic year 2010 – 11)

Course Structure

Course I : Research methodology 100 marks (05 credits)

Course II : Advances in Chemistry 200 marks (10 credits)

Course III : Seminar, Field work & Review Writing 100 marks (05 credits)

University of Pune**Department of Chemistry****Syllabus for M.Phil. / Ph.D. course in Chemistry to be implemented from academic year 2010 - 11****Course I : Research methodology****100 marks (05 credits)**

Fundamental Laboratory Techniques : Basic principles, Health and safety, working with liquids, Basic laboratory procedures I, Basic laboratory procedures II, Principles of solution chemistry, pH and buffer solutions (Ref. 1. Chapters 1 to 7 : pages 03 to 62)

The investigative approach : Making and recording measurements, SI units and their use, Scientific method and design of experiments, Project work (Ref. 1. Chapters 8 to 11 : pages 65 to 83)

Analysis and presentation data : Using graphs, Presenting data in tables, Hints for solving numerical problems, Descriptive statistics, choosing and using statistical tests, drawing chemical structures, chemometrics, computational chemistry (Ref. 1. Chapters 37 to 44 : pages 251 to 295)

Information technology and library resources : The Internet and World Wide Web, internet resources for chemistry, using spreadsheets, word processors, databases and other packages, finding and citing information (Ref. 1. Chapters 45 to 49 : pages 299 to 321)

Communicating information : General aspects of scientific writing, writing essays, reporting practical and project work, writing literature surveys and reviews, organizing a poster display, giving an oral presentation examinations (Ref. 1. Chapters 50 to 56 : pages 325 to 354)

Chemical safety and Disaster Management :

(a) **Emergency response** : chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency accident reporting

(b) General safety : General safety and operational rules, safety equipments, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass wares, centrifuge safety, treated biomedical wastes and scientific ethics.

Research problem : meaning of research problems, sources of research problems, criteria / characteristics of a good research problem, errors in selecting a research problem.

Hypothesis : Meaning, types of hypothesis.

Developing a Research Proposal : Format of research proposal, individual research proposal and institutional proposal.

Research Report : Format of the research report, style of writing the report, references and bibliography.

Books :

1. 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)
2. OSU safety Manual 1.01.
3. Research Methodology. Methods and Techniques : C. R. Kothari,
4. Tests, Measurements and Research Methods in Behavioural Sciences : A. K.Singh.

Course II : Advances in Chemistry**200 marks (10 credits)****Student can opt any one of the following****(I) Advances in physical chemistry (10 credits)****Part A 100 Marks (5 credits)**

Analytical Techniques : Any Five

Principle, Instrumentation, Applications, Analysis and Interpretation of the data for the following techniques:

UV-Visible Spectrophotometry, IR, GCMS, TG-DTA, Nuclear Analytical Techniques, Fluorimetry, NMR, AAS, ICPAES, XRD. Use of Fortran and C ++ programs

Part B 100 Marks (5 credits)

Any two of the following modules:

- a. Chemistry of Materials
- b. Molecular Modeling and Computational Chemistry

Methods based on Hartree-Fock, Configuration Interaction

Deriving one and two electron properties

Semi-empirical methods

Coupled Cluster theory

Density functional theory, TDDFT

Molecular Dynamics

Drug Discovery and Drug Design

- c. Electrochemistry and Electroanalytical Techniques
- d. Environmental Chemistry
- e. Advanced Topics in Kinetics and Thermodynamics
- f. Radiation and Photochemistry

References

1. Essentials of Nuclear Chemistry, H. J. Arnikaar, Wiley Eastern Limited, 4th Edition.(1995)
2. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy and J. M. Miller, John Wiley (1981)
3. Introduction to Radiation Chemistry, J. W. T. Spinks and R. J. Woods, John Wiley (1990)
4. Introduction to Nuclear Physics and Chemistry, B.G. Harvey, Prentice hall (1963).
5. Sourcebook on Atomic Energy-S. Glasstone, Van Nostrand Company (1967)
6. Radiochemistry and Nuclear methods of analysis-W.D.Ehman and D.E. Vance, John Wiley (1991)
7. Fundamentals of photochemistry by K.K.Rohatgi-Mukherjee New Age International Publishers Revised Edition (Reprint 2003)
8. Chemistry and light by Paul Suppan, The Royal Society of Chemistry
9. Introduction to Instrumentation Analysis by R.D. Braun Pharma Med Press
10. Introduction to Instrumental Analysis- R. D. Braun, Pharmamed Press, Indian Reprint (2006)
11. Principles of Instrumental Analysis, 5th edition- D.A. Skoog, F.J. Holler, T.A. Nieman, Philadelphia Saunders College Publishing (1988)
13. Principles of activation analysis - P. Kruger , John Wiley (1971)
14. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)
15. Modern Quantum Chemistry, A. Szabo and N.L. Ostlund, Dover, New York (1996).
16. Approximate Molecular Orbital Theory, J.A. Pople and D.L. Beveridge, McGraw Hill, New York (1971)
17. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford University Press, Oxford (1989).
18. Molecular Modeling, A. Leach, Longman, Landon (1996).
19. Computers and Common Sense R. Hunt and Shelley, Prentice Hall, New Delhi (1998)
20. Computer Programming in Fortran-90 V. Rajaraman, Prentice Hall, New Delhi (1990)
21. Computer and Chemistry: introduction to programming and numerical methods T. R. Dickson, Freeman (1968)
22. Computer programs for chemistry D. F. Detar W. A. Benjamin Inc, New York Vol. 1-3 (1968-69)
23. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)

24. Electrochemical Methods second edition, A.J. Bard and L.R. Faulkner, John Wiley and Son (2001).
25. Molecular Modelling, A. Leach, Longman, London (1996).
24. Introduction to Computational Chemistry, F. Jensen, John Wiley, New York (1999).
24. Computational Chemistry (Theories and Models), D. Cramer, John Wiley, New York (2002).
24. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).
25. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).
30. Bard, A. J. Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., John Wiley & Sons: New York, 2002.
31. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
32. Antropov, L.I. *Theoretical Electrochemistry* Physical Principles of Electron Microscopy: An Introduction to TEM, SEM and AEM by Ray F. Egerton Springer
33. Handbook of Instrumental Techniques for Analytical Chemistry Editor by Frank Settle Pearson Education (Singapore).
34. Nanoscale Materials in Chemistry Editor by Kenneth J. Klabunde John Wiley & Sons

OR**(II) Advances in Inorganic chemistry 200 Marks (10 credits)****Part A 100 Marks (5 credits)**

1. Chemistry of metals / non-metals (minimum two)
2. Chirality in transition metal Chemistry
3. Biological Inorganic Chemistry
4. Bioorganometallic chemistry
5. Physical methods in Inorganic Chemistry (a) Raman spectroscopy
(b) XPS spectroscopy

Part B 100 Marks (5 credits)

1. Nanomaterials and nanostructures
2. Chemistry of materials (a) Magnetic oxides
(b) Superconductors
(c) Ferroics
3. Surface Science and heterogeneous catalysis
4. Environmental Toxicants
5. Modern Analytical Methods : (a) Inductively coupled plasma spectrometry
(b) Advanced separation techniques :
 - i. High performance liquid chromatography
 - ii. Gas chromatography for separation and Mass Spectrometry (GC/MS)

Books:

1. Comprehensive Inorganic chemistry, J. C. Bailar, H. J. Emeleus, Sir R. Nyholm, R. F. Tortman- Dickenson (Pergamon Press, 1973) Volume 1 to 5.
2. Chirality in transition metal Chemistry, Hani Amouri and Michel Gruselle (Wiley,2008)
3. Biological Inorganic Chemistry, Robert R. Crichton
4. Bioorganometallic chemistry, Volume Editor G. Simonneaux (Springer, 2009)
5. Physical methods for chemists R.S. Drago (Saunders Co. 1992)
6. Nanomaterials and nanostructures, Laura Costlow, April Feter (Dominant Publisher,2007)
7. Inorganic Material Chemistry, M. T. Weller (Oxford,1994)
8. Catalysis : Principles & Applications, B. Vishvanathan, S. Sivasankar and A.V. Ramaswamy (Narosa Publication House, New Delhi 2004)
9. Introduction to Zeolite Science & Practice, H. Van Bekkum, E.M. Flanigen, P.A. Jacobs & J.C. Jansen (Elsevier Publication, Amsterdam, 2001)
10. Environmental Toxicants, Morton Lippmann (Wiley International, 2000)
11. Magnetic Oxides, Part 1 and 2., D. J. Craik (John Wiley and Sons,New York, 1975)
12. Chemistry and Structural Aspects of high Tc superconductors, C. N. R. Rao (World Scientific, Singapore, 1998)
13. Inductively coupled plasma spectrometry and its applications, Steve J. Hill (Sheffield Academic Press, 1999)
14. High Performance liquid chromatography : Principles and Methods, Elena D. Katz (John Wiley & Sons Ltd. 2009)
15. GC/MS, A Practical User Guide : Marvin McMaster & Christopher McMaster (Wiley – VCH 1998)
16. Introduction Raman Spectroscopy (2nd Edition) John R. Ferraro, Kazuo Nakamoto & Chris W. Brown (Academic Press, Elsevier, 2005)

OR

(III) Advances in Organic chemistry 200 Marks (10 credits)

Part A : Advances in Organic Chemistry 100 Marks (05 credits)

1. Advances in C-C bond formation 20 lectures
2. Advances in C-Heteroatom bond formation 10 lectures
3. Retrosynthetic analysis and selected total synthesis 20 lectures
4. Biomolecules and biological activity determination. 10 lectures

Part B : Reaction Mechanism, Stereochemistry & Spectroscopy 100 Mark(5 credits)

1. Advanced stereochemistry and asymmetric synthesis. 15 lectures
2. Reactive Intermediates, reactions and Rearrangements 15 lectures

3. Spectroscopy

- i. Introduction to IR, UV, ¹HNMR, ¹³CNMR, Ms techniques 05 lectures
- ii. Introduction to COSY, HSQC, HMBC, NOESY, ROSEY 10 lectures
- iii. Techniques like X-ray, LCMS, GCMS, HPLC, HRMS 05 lectures
- iv. Application of the spectral and analytical techniques 10 lectures
for structure determination.

Books:

1. Advanced Organic Chemistry, Fourth Edition, Part A and B
F.A.Carey and R.J.Sundberg

2. Organic Chemistry

Clayden, Greeves, Warren and Wothers

3. Advanced organic chemistry by J. March, 6th Ed.

4. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed.

(Harcourt college publishers).

5. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster,

6th Ed. John Wiley and Sons.

6. Stereochemistry of carbon compounds - E. L. Eliel

7. Some modern methods of organic synthesis – W. Carruthers (Cambridge)

8. Organic synthesis – M. B. Smith

Course III : Seminar, Field work & Review Writing* 100 marks (05 credits)

1. **Seminar** : Seminar to be delivered on a relevant theme (**01 credits**)
2. **Field Work** : Visit to industry/National institutes and interaction with experts. (Report to be submitted) (**01 credits**)
3. **Review** : Preparation and submission of review article based on research papers addressing a contemporary research problem. (**02 credits**)
4. **Other activities** : Attending National / International workshop / Symposium / Conferences or participation for oral / poster presentation or interaction with M.Sc. students for problem solving approaches / Work of Nobel laureates in last ten years in Science. (**01 credits**)

* Above topics shall be prepared in consultation with research guide
