SHIVAJI UNIVERSITY, KOLHAPUR

Syllabi of Ph. D. /M. Phil. Course Work

in

Chemistry

DEPARTMENT OF CHEMSTRY
(UGC-SAP & DST-FIST Sponsored)
June, 2011

Shivaji University, Kolhapur

M. Phil./Ph. D. Course Work

New Syllabus

A] **Ordinance/Rules/Regulations** **:** As applicable to M. Phil. /Ph. D. Programme.

A candidate who registers as a regular student for Ph. D. will have to complete the course work of one semester duration within two years.

a) A candidate who has obtained M.Phil. Degree or completed his/her theory course as per the UGC Rules and Regulation shall be exempted from the Ph.D. Course Work.

b) A candidate who has passed M.Phil. Degree after 2009 and who has completed prerequisite course on quantitative methods and computer application conducted by Shivaji University will be exempted from Ph.D. course.

B]

1. **Subject** **:** Chemistry

Optional/Compulsory **:** Compulsory
under the Faculty of

2. YEAR OF MPLEMENTATION **:** New course work will be implemented from June 2011

onwards.

3. PREAMBLE :

Total No. of Papers : 3

Work load for each paper: 60 hrs

Maximum marks per paper : 100

Total marks **:** 300

Title of papers:

Paper-I : Research Methodology and Computer Applications in Chemistry (Compulsory)

Paper-II : Recent Trends in Chemistry(Compulsory)

Paper-III : Selected Topics in Organic Chemistry (Optional)

Paper-III : Selected Topics in Inorganic Chemistry (Optional)

Paper-III : Selected Topics in Physical Chemistry (Optional)

Note: Candidate has to select any one paper out of three elective .papers

4. **DURATION** **:** The M. Phil. programme shall be a full time regular course. The duration of M. Phil. programme shall be of One year.

5. PATTERN OF EXAMINATION: Annual in respect of M.Phil and Semester in respect of Ph.D.

FEE STRUCTURE **:** As applicable to regular/ Self Supporting Course

i. Entrance Examination Fee : (If applicable) Rs (Non refundable)

ii. Course Fe :

Particulars	Rupees
Tuition Fee	Rs.
Laboratory Fee	Rs.
Internet Fee	Rs.
Library Fee	Rs.
Annual/Semester fee-per student	Total Rs.

6. **ELIGIBILITY FOR ADMISSION :** As per eligibility criteria prescribed for each course and the merit list in the qualifying examination.

7. **MEDIUM OF INSTRUCTION :** The medium of instruction shall be in English or Marathi. (as applicable to the course/programme concerned.)

8. STRUCTURE OF THE COURSE WORK FOR M. Phil. /Ph. D. :

NO. OF PAPERS : THREE

Sr. No.	Subjects/Papers	Marks
1.	Research Methodology and Computer Applications in Chemistry (Compulsory)	100
2.	Resent Trends in Chemistry	100
3.	Paper-III(A) : Selected Topics in Organic Chemistry (Elective) Paper-III(B) : Selected Topics in Inorganic Chemistry (Elective)	100 (80 + 20)

	Paper-III©: Selected Topics in Physical Chemistry (Elective)	
	Total	**300**

9. **SCHEME OF TEACHING AND EXAMINATION** **:** The scheme of teaching and examination should be given as applicable to the course/paper concerned.

Sr. No.	**Subjects/Papers (Hrs/Week**				**Examination Schemes (Marks)**		
	L	**T**	**P**	**Total**	**Theory**	**Term Work**	**Total**
1	4	-	-	4	100	-	100
2	4	-	-	4	100	-	100
3	4	-	-	4	100	-	100

10. SCHEME OF EXAMINATION :

- **The examination shall be concluded at the end of each Term/each academic year.**
- **The Theory paper shall carry 100 marks.**
- **The evaluation of the performance of the students in theory Papers shall be on the basis of Annual Examination of 300 marks.**
- **Question Paper will be set in the view of in accordance with the entire syllabus and preferably covering each unit of syllabi.**

11. **STANDARD OF PASSING** **:** As Prescribed under rules and regulation for each degree/programme
Separate heads of passing with minimum 40 marks in each paper

12. NATURE OF QUESTION PAPER : AND SCHEME OF MARKING (Unit wise weightage of marks should also be mentioned)

:a) Paper-I 100 marks

i) Question paper consists of five questions each of 20 marks.
II) All questions are compulsory
iii) Q.1 is objective.
iv) Q.2 to Q.5 should include internal options.

b) Paper-II 100 marks

i) Question paper consists of five questions each of 20 marks.
II) All questions are compulsory
iii) Q.1 is objective.
iv) Q.2 to Q.5 should include internal options.

c) Paper-III 80 marks University examination + 20 marks Seminar on review of published research work

i) Question paper consists of five questions each of 16 marks.
II) All questions are compulsory
iii) Q.1 is objective.
iv) Q.2 to Q.5 should include internal options.

12. EQUIVALENCE IN ACCORDANCE WITH TITLES AND CONTENTS OF PAPERS (FOR REVISED SYLLABUS) :

Equivalence:

Sr. No.	Title of Old Papers	Titles of New papers
1.	Paper-I: General Chemistry	Paper-I : Research Methodology and Computer Applications in Chemistry
2.	Paper-II: i) Recent Advances in Inorganic Chemistry ii)Advanced Organic Chemistry iii) Quantum Chemistry, Thermodynamicsand Photochemistry iv) Analytical and Industrial Chemistry v) Advanced Polymer Chemistry	Paper-II: Recent Trends in Chemistry:
3.	Paper-III(A):Structural Inorganic Chemistry Paper-III(B):Advances in Solid State Chemistry Paper-III©:Advances in Separation Sciences.	Paper-III:Selected Topics in Inorganic Chemistry
4.	Paper-III(A):Physicoorganic Chemistryc Paper-III(B):Synthetic Organic Chemistry	Paper-III:Selected Topics in Organic Chemistry
5.	Paper-III(A):Molecular Spectroscopy Paper-III(B):Selected Topics in Solid State Chemistry Paper-III(C):Electrochemistry, Chemical Kinetics and Catalysis	Paper-III:Selected Topics in Physical Chemistry

13. SPECIAL INSTRUCTIONS, IF ANY. -----

NEW/REVISED SYLLABUS FOR

M. Phil. / Ph. D. Course Work
(Introduced from June, 2011 onwards)

Paper-I : Research Methodology and Computer Applications in Chemistry

UNIT-I : Computer Applications:

Use of Computer Programs: (15)

1. The students will learn how to operate a PC and how to run standard programs and packages. Execution of linear regression, X-Y plot, numerical integration and differential as well as differential equation solution programming, Monte Carlo and Molecular dynamics. Programs with data preferably from physical chemistry laboratory. Introduction to computation tools such as Molecular modeling, molecular dynamics simulations, energy minimization and conformational search methods, use of molecular dynamics for normal mode analysis, free energy calculations and conformational analysis.

2. Computational methods for drug discovery.

3. Chemical information, structure elucidation, synthesis design, simulation of reaction, physicochemical data, molecular modeling, molecular graphics, data banks.

4. Chemo metrics – Computer based laboratory, statistics and data interpretation, Computer based information systems.

UNIT-II : Quantitative Techniques: (15)

Classification of quantitative methods, General steps required for quantitative analysis, reliability of the data, classification of errors, accuracy, precision, statistical treatment of random errors, the standard deviation of complete results, error proportion in arithmetic calculations, Uncertainty and its use in representing significant digits of results, confidence limits, Estimation of detection limit.

UNIT-III : Research Methodology: (15)

Introduction to research methodology, design and implementation of research methods, types of research, the research process, formulating, reviewing the literature.

UNIT-IV : Literature Searching and Writing Reports: (15)

Literature Searching

On-line searching, Database, Scifinder, Scopus, CA on CD

Locating research article, Citation Index, Impact Factor

Writing scientific report :

Planning, preparation, draft, revision and refining; writing project prosal to funding agency, Paper writing for International Journals, submitting to editors. Conference presentation, preparation of effective slides and presentation.

References:

1) Fundamentals of analytical Chemistry by D. A. Skoog, D. M. West and F. J. Hooler.

2) Quality in the Analytical Chemistry Laboratory by R. D. Treble and D. G. Holcombe.

3) Molecular dynamics simulations elementary methods by J. M. Haile.

4) The art of molecular dynamics simulations by D. C. Rapaport.

5) Introduction to computational chemistry by F. Jensen.

6) Molecular modeling principles and applications by A. R. Leach.

7) Computer Education by Prof. Lalini Varanasi, Prof. V. Sudhakar and Dr. T. Mrunalini, Neelkamal Publications PVT. LTD.

8) Basic Computing Principles by B. West, BPB Publications, New Delhi 1992

9) Essentials of computational chemistry by C. J. Cramer.

10) Practical Research Methods, Catherine Dawson, UBS Publishers Distribution, New Delhi 2002.

11) Research Methodology – Methods and Techniques, C. R. Kothari, Wiley Easter Ltd, New Delhi 1985.

12) Research Methodology – A Step by step Guide for Beginners 2nd edn. Kumar Ranjit, Pearson Education, Singapore, 2005.

13) Introduction to Research and Research Methodology M. S. Sridhar.

14) The Information Specialist's Guide to Searching & Researching on the Internate & the World Wide Web by Ernest Ackermann, Karen Hartman, Fitrzroy Dearborn Publishers, London.

15) Learnig to Use the World Wide Web, Ernest Ackermann, BPB Publications.

Paper-II : Recent Trends in Chemistry:

Unit-I : NMR, IR and Mass Spectroscopy: (15)

a) IR spectroscopy: Applications of IR in analysis.

b) NMR spectroscopy: Chemical shifts, and coupling constant, Introduction of NOE, DEPT and 2D NMR, ^{13}CNMR and its applications.

c) Mass spectroscopy: Mass spectral fragmentation of complex molecules and its applications.

d) Combined spectroscopic problems based on IR, NMR, and mass spectral data.

Unit-II : X-ray Diffraction, XPS, EDX and TEM : (15)

Principle instrumentation and application of X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and electron spectroscopy for chemical analysis (ESCA), transmission electron microscopy (TEM), Scanning electron microscopy (SEM).

Unit-III: Fluorescence Spectroscopy: (15)

Introduction, Phenomenon and characteristic of fluorescence, fluorescence life time. Fluorescence quenching, types of quenching processes, Instrumentations, experiments for fluorescence quenching measurements, Applications in development of analytical techniques and understanding the molecular interactions.

Unit-IV: Hyphenated Techniques: (15)

A] Basics of analytical Method development and Validation study

General approach to method development and validation, Study of validation parameters following ICH guidelines, Accuracy, Precision, Linearity, Range, Limit of detection(LOD), Limit of quantification(LOQ), System suitability, Stability, Ruggedness, Robustness

B] High Performance Liquid Chromatography (HPLC)

Introduction, scope, principle and instrumentation, Column type, efficiency, separation parameters, Supercritical fluid chromatography (SFC) and extraction (SEC) and Applications

C] Hyphenated Methods

Introduction, principle, scope, instrumentation and applications of LC-MS, GC-MS, IC-MS, HP-TLC, and ICP-MS

References:

1) Silverstein and Basallar: Spectroscopic identification of organic compounds.

2) V. M.Parikh: Absorption spectroscopy of organic compounds. (J. Wiley)

3) D.W. Williams and Flemming: Spectroscopic methods of organic compound.

4) J.R. Dyer: Application of absorption spectroscopy of organic compounds:

5) Analytical Chemistry (JW)G.D.Christain

6) Instrumental Methods of Analysis: Chatwal & Anand

7) Principles of Instrumentals Analysis: D.Skoog & West

8) Introduction to Chromatography: Bobbit

9) Chemical Instrumentation: A Systematic Approach-H.A.Strobel

10) Treatise on Analytical Chemistry: Vol. , I-VII I.M.Kilthoff,

11) Applications of Spectroscopy Techniques in Organic Chemistry: P.S.Kalsi

12) A text Book of Qualitative Inorganic Chemistry: A.I.Vogel

Paper-III: Selected Topics in Inorganic Chemistry

Unit-I: Inorganic Nanomaterials and Their Applications: (15)

Introduction to nanomaterials, Physicochemical properties of nanomaterials (Optical, Electrical, Electronic Redox, Mechanical, Magnetic and catalytic).Synthesis and Preparation of nanostructured oxides and chalcogenides. Influence of nanomaterials on health, communication, Energy, Environment, safety, security and defence. Special applications of nanomaterials, sensor, energy storage, nanoelectronics and computing structural materials (Nanocomposites) catalysis communication, nanomedicine.

Advanced nanomaterials , Si, C, Ag, Au, Pt nanoparticles.

Unit-II: Inorganic Materials and Nanotechnology Instrumentation: (15)

Advanced inorganic materials, TiO2, WO3, ZnO and metal chalcogenides, ceramics, ferrites, magnetic, non-linear optics in molecular materials

Instrumentation:- Atomic force microscopy (AFM), Raman spectroscopy, Scanning tunneling microscopy, electron spectroscopy for chemical analysis (ESCA)

Unit-III: Co-Ordination Organometallic Complexes and Characterization Techniques: (15)

Introduction to co-ordination complexes, synthetic methodology, ligational behavior types of ligands, spectroscopic characterization of complexes, magnetic and electrochemical behavior of complexes.

Organometallic compounds: Types, synthetic methodology with special reference to metal acetylide and carbonyl compounds, spectroscopic characterization, applications of co-ordination and organometallinc compounds.

Unit-IV: Reverse Phase Extraction Chromatography (RPEC): (15)

Extraction chromatography, theoretical aspects of extraction chromatography, correlation between solvent extraction chromatography, chromatography inert support stationary phases, applications of extractions chromatography.

Reference books:

1. Nanomaterials, B. Viswanathan.
2. Nanotechnology applications, Daniel Minoli.
3. Nanocrystalline oxide materials, K. C. Patil, M. S. Hegade, Tanu Rattan, S.T. Aruna.
4. Synthesis, properties and applications of oxide nanomaterials, Jose A. Rodriquez, M. F. Garcia.
5. Trends in Chemistry of materials, C. N. R. Rao.
6. Inorganic Chemistry, Hollman Wiberg.
7. Instrumentation methods of Chemical analysis, H. Kaur.
8. Modern Raman Spectroscopy, Eulem Smith, Geofferey Dent.
9. Organometalic Chemistry, Paulson, Arnold.
10. Organometalic Chemistry, Rochow, Reinhold.
11. Organometalic Chemistry, Reinhold, Zeiss.

12. Optoelectronic properties of Inorganic compounds, D. Max Roundhill and John P. Fackler.

Paper-III: Selected Topics in Organic Chemistry

UNIT-I: New synthetic methodologies and applications of reagents: (15)

Microwave and ultrasonic methods of synthesis, biocatalysts and biotransformations, phase transfer catalysts, electro-organic synthesis, Ionic liquids,Enantio and diastereoselective synthesis use of oxone, hyper valent iodine reagents, and complex metal hydrides, Organometilics compounds of Cu, Ni, Se Co and Organoboranes.

UNIT-II : Designing of Organic Synthesis (Retrosynthesis): (15)

a) Retrosynthesis of heterocycles, agrochemicals, natural products, and perfumery compounds.
b) Synthesis and applications of the following drugs: Cardiovascular, antidiabetics, antineoplastics, and antiviral drugs.
c) Computer aided drugs designing and molecular modeling

UNIT-III: Organic Photochemistry: (15)

a) Photochemical processes, photo reactions of dienes, arenes and carbonyl compounds. Reactivity of singlet and triplet oxygen, Photorearrengements, Applications of photoreactions in laboratory and industrial synthesis.
b) Stereochemistry of Chlolestane, Yohimbine and Reserpine.

.UNIT-IV: Synthesis of Natural Products: (15)

a) β-Vetivone
b) Solavetivone
c) Nootkatone
d) (+-)Cuprene(Kametani synthesis and Demayo synthesis)
e) Laurene

f) (+-)Acorinone (Trost synthesis and Wolf synthesis)

g) Juvabione

h) Cis-Jasmone

i) Synthesis of prostaglandins

Reference books:

1] H.O.House: Modern Synthetic Reaction.

2] M.B.Smith: Principles of Organic Synthesis

3] (McGraaw Hill) Hendrikson, Cram and Hammond: Organic Chemistry

4] E.L. Eliel: Stereochemistry of Carbon Compounds

5] D. Nasipuri: Stereochemistry of Organic Compound.

6] S.Warren: Designing of Organic Synthesis

7] Warren ant Wyatt: Organic Synthesis: Strategy and Control

8] Apsimon: The Total Synthesis of Natural Products.

9] I. Finar: Organic Chemistry Vol. II and I

10] J. Kagan: Organic Photochemistry

11] H.Arora: Organic Chemistry and Pericyclic Reaction.

12] J. Coxon and B. Hallon: Organic photochemistry Cambridge University Press.

(Studies on use of computer software's related to above techniques is expected)

Paper-III : Selected Topics in Physical Chemistry

Unit-I : Preparation of Materials and applications: **(15)**

a)Thin films and Langmuir- Blodgett Films:
Preparation techniques; sol - gel, spin coating, Langmuir- Blodgett (LB) photolithography, properties and applications of films.

b) Materials of Solid State Devices:
Organic and inorganic materials for rectictifiers, transistors, capacitors and their applications in optoelctronic and photovoltaic devices.

Unit-II : Kinetics of redox reactions: **(15)**

Outer and inner sphere reactions, kinetics and mechanism of oxidation reactions involving chromium, ruthenium and silver(III).

Kinetics of catalyzed reactions: Homogeneous and heterogeneous. Positive, negative and auto catalysed reactions. Induced reactions, promoters and poisons.

Theories of catalysis: intermediate compound formation and adsorption theory, characteristic of catalytic reaction and activation energy of catalyzed reactions.

Micellar Catalysis: Models for micellar catalysis(Menger & Portony, Sepulveda, Berezin, Piszkiewicz and Raghavan & Srinivasan Models), Phase transfer catalysis, General mechanism, difference between phase transfer and mecellar catalysis.

Unit-III : Organic Nanomaterials and applications: (15)

Introduction to nanomaterials, preparation methods, properties of nano materials, electrical and optical properties, applications of organic NP in analysis and devices.

Unit-IV: Thermodynamic and Dielectric Properties of Liquids and Solutions: (15)

Structure of liquids, relationship between structure and the thermodynamics properties, molecular theory of monoatomic and polyatomic liquids, thermodynamics of phase equilibria, statistical molecular description of phase transitions, chemical potential and partial molar quantities, mixing and excess thermodynamic properties of mixtures, statistical mechanical theories of nonelectrolyte and electrolyte solutions, influence of solute on structure of water, structure of water near a surface

Static dielectric constant: Dipolar interactions, dipolar molecules in gases and in dilute solutions. Debye equation and its generalizations, Structure and dielectric properties, methods for determination of dipole moments, Clausius-Mossotti equation, dielectric loss, cole-cole plots, dielectric relaxation.

(Studies on use of computer software's related to above techniques is expected)

REFFERNCE BOOKS:

1. Solid State Physics, N. W. Ashcrott and N. D. Mermin, Saunders College
2. Material Science and Engineering, An introduction , W. D. Callister, Willey.
3. Principals of Solid State, H. V. keer, Willey Eastorn.
4. Materials Science , J. C. Anderson , K. D. Leaver, J. M. Alexander and R. D. Rawlings, ELBS
5. Chemical Kinetics by K. J. Laidler.
6. Kinetics and Mechanism by A. A. Frost and R. G. Pearson
7. Micellar effect on the kinetics and mechanism of chromium(VI) oxidation Of organic substrates By Asim K. Das, Coordination Chemistry Reviews,Vol 248, p 81-89 (2004).
8. Some aspects of electron transfer reactions involving organic molecules by B.Sethuram, Allied Publishers, 2003.
9. Surfactants and polymers in aqueous solution by Bo Jonsson, Bjorn Lindman, Krister Holmberg and Bengt Kronberg, John-Wiley & Sons, 1998.
10. Nanomaterials, B. Viswanathan.
11. Nanotechnology applications, Daniel Minoli.
12. Nanocrystalline oxide materials, K. C. Patil, M. S. Hegade, Tanu Rattan, S.T. Aruna.
13. Synthesis, properties and applications of oxide nanomaterials, Jose A. Rodriquez, M. F. Garcia.
14. Trends in Chemistry of materials, C. N. R. Rao.
15. R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, 2nd Ed., Oxford University Press, New York, 2000.
16. A. Ben-Naim, *Water and Aqueous Solutions*, Plenum Press, New York, 1974.
17. D. A. McQuarrie, *Statistical Mechanics*, Harper and Row Ltd., New York, 1976.
18. Y. Marcus, *Introduction to Liquid State Chemistry*, Wiley, New York, 1977.

19. K. S. Pitzer, *Thermodynamics*, 3rd Ed., McGraw Hill, New York, 1995.

20. H. Frohlich, *Theory of Dielectrics: Dielectric Constant and Dielectric Loss*, 2nd Ed. Oxford University Press, New York, 1958.

21. V. I. Gaiduk, *Dielectric Relaxation and Dynamics of Polar Molecules*, World Scientific Publishing Co., Singapore, 1999.

22. J. B. Hasted in *Water: A Comprehensive Treatise*, edited by F. Franks (Plenum Press, New York, 1973), Vol. II.

23. Chemical Kinetics by Keith J. Laidler, third edition, Pearson(2004)

24. Chemical Kinetics and Reaction Dynamics by Santosh K. Upadhyay, Anamaya (2008).

25. Some Aspects of Electron Transfer Reactions Involving Organic Molecules by B. Sethuram, Allied Publishers (2003).

26. Mechanism of Inorganic Reactions by F. Basolo and R. G. Pearson, John Wiley(1967).