SYLLABUS

M. Phil. (Chemistry)

DEPARTMENT OF CHEMISTRY
PONDICHERRY UNIVERSITY
PONDICHERRY – 605 014

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PONDICHERRY UNIVERSITY

The Department of Chemistry belongs to the School of Physical, Chemical and Applied Sciences and it offers different programs leading to M. Sc. Integrated Program in Chemistry, M. Sc. Chemical Sciences, M. Phil. Chemistry and Ph.D. degrees. Students are admitted to M.Sc. Integrated program in Chemistry after 10+2 system of schooling, M.Sc. Chemical Science after three year under-graduation, M.Phil. Chemistry and Ph.D. after two year post-graduation. Details of eligibility criteria are available in the information brochure. Normally students are expected to take 10 semesters for M.Sc. Integrated program, 4 semesters for M.Sc. and 2/3 semesters for M.Phil. to complete requirements for the degree. The department follows Choice Based Credit System (CBCS). The students are expected to earn at least **192** credits for M.Sc. integrated program, **72** credits for M.Sc. and **36** credits for M.Phil. It is mandatory for the students to clear all the hard core courses and exercise selection from among the soft-core courses offered by the Department. Apart from the courses taken within the department, students are expected to take optional courses from among the breadth courses offered by sister departments in the University.

M.Sc. integrated and M.Sc. Chemcial Sciences students are expected to do project work spanning one semester in the final year. In addition, the students also do advanced practical. Both the advanced practical and the project courses are faculty oriented. Students are tuned to research in chemistry under the guidance of the selected faculty member.

The Department strives to provide broad based education in Chemistry at graduate, post-graduate and research levels. The students are expected to evolve interdisciplinary attitudes while going through various programs of the Department and the University.

M. Phil. Chemistry
Course Structure

1st Semester:

1 Chemical Bonding And Reactivity - CHEM 660; 6 Credits; HC
Any **Two** of the following Three Courses:
2 Physical Methods in Inorganic Chemistry - CHEM 602; 6 Credits; SC
3 Advanced Topics in Organic Chemistry - CHEM 622; 6 Credits; SC
4 Theoretical and Computational Chemistry - CHEM 662; 6 Credits; SC

Number of Credits for the Semester = 18

2nd and 3rd Semesters:

1 Dissertation - CHEM 702; 15 Credits; HC
2 Viva – Voce - CHEM 703; 3 Credits; HC

Number of Credits for the Semester = 18

M.PHIL COURSES

CHEM 660 CHEMICAL BONDING AND REACTIVITY

Pre-requisite: M. Sc. Chemistry / Chemical Sciences; **HC** **Credits: 6**

UNIT – I

Elements of Quantum Chemistry

Basic quantum mechanics, Atomic structure, diatomic molecules, MO and VB theories – polyatomic molecules - hybridization, delocalised systems: HMO, EHT methods – SCF MO theory – semi-empirical methods – charge density – bond orders – reactivity indices – frontier electron theory – recent developments in reactivity models.

UNIT – II

Bonding & reactivity of Transition metal complexes:

CFT, LFT, angular overlap model, electronic spectra and magnetic properties, exchange interactions, EPR – reactions of coordination compounds – electron transfer reactions

UNIT – III

Reactivity of Organic Molecules. Pericyclic Reactions:

Frontier orbitals in conjugated systems (up to 6 electrons) – pericyclic reactions – Woodward Hoffmann rules – Frontier orbital approach – correlation diagrams – Mobius Huckel approach – cycloaddition reactions – sigmatropic rearrangement – electrocyclic ring closure and opening reactions – application of pericyclic reactions in organic synthesis

Recommended Books:

1. M. Karplus and Porter, Atoms & Molecules
2. J. M. Murrell, S. F. A. Kettle & Tedder, Valence Theory
3. P. W. Atkins, Molecular Quantum Mechanics
4. Woodward & Hoffmann, The Conservation of Orbital Symmetry, Academic Press, 1970
5. I. Fleming, Frontier Orbitals & Organic Chemical Reactions, John Wiley, 1976
6. B. N. Figgis, Ligand Field Theory, Wiley Eastern
7. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1986.

CHEM 602 PHYSICAL METHODS IN INORGANIC CHEMISTRY

Pre-requisite: M. Sc. Chemistry / Chemical Sciences; **SC** **Credits: 6**

UNIT – I

Magnetic Susceptibility:

Basic Theory, spin only moments, spin orbital interactions, temperature dependence of magnetic susceptibility – methodology: Guoy, Faraday, VSM, SQUID.

UNIT – II

Spectral Techniques:

NMR of paramagnetic molecules, contact and dipolar shifts, ^{15}N, ^{19}F, ^{91}P NMR, NMR of heavy nuclei – Mossabauer spectroscopy: basic principles, instrumentation and applications – ESCA – Auger – EXAFS – XANES.

UNIT – III

EPR of Transition metal ions:

Spin Hamiltonian, spin-orbital coupling, g and A matrices, solutions to S=1/2 systems in various ligand fields, d^9, d^1, d^5 systems, S>1/2 systems, zero-field splitting – single crystal and powder spectra – spin-lattice and spin-spin relaxation.

Recommended Books:

1. A. Abragam and B. Bleaney, Electron Paramagnetic Resonance, Dover, 1986
2. R. S. Drago, Physical Methods in Chemistry, Saunders, 1987

CHEM 622 ADVANCED TOPICS IN ORGANIC CHEMISTRY

Pre-requisite: M. Sc. Chemistry/Chemical Sciences; **SC** **Credits: 6**

UNIT – I

Recent Advances in Structure Determination of Organic Molecules:

Spectrometric methods in organic molecules – pulsed NMR techniques (^{1}H and ^{13}C) – application of 2-D NMR – mass spectrometric techniques, parent and daughter ion analysis – problem solving exercises

UNIT – II

Molecular Recognition:

Designed Host-Guest relationships (based on oxygen, nitrogen and aromatic macrocycles) – molecular recognition in biochemical process – Thermodynamics, kinetics and stereochemistry in molecular recognition

UNIT – III

Topics in Stereochemistry:

Conformational flexibility in large rings (seven to eleven) – asymmetric synthesis – application of chiral auxiliaries in asymmetric synthesis

Recommended Books:

1. A. W. Derome, Modern NMR techniques for Chemistry Research, Pergamon press, 1987
2. W. Kemp, NMR in chemistry, a multinuclear introduction, MacMillan, London, 1986
3. P. W. McLafferty, Interpretation of Mass spectra, University Science Books, 1980
4. G. Van Binst, Design and Synthesis of organic molecules based on molecular recognition, Springer Verlag, 1986
5. R. M. Izatt, J. L. Christensen Eds., Synthesis of Macrocycles, The design of selective complexing reagents, John Wiley and sons, New York 1987.
6. J. P. Collman et. al., Principles and application of organometallic transition chemistry, 1987.

CHEM 662 THEORETICAL AND COMPUTATIONAL CHEMISTRY

Pre-requisite : M. Sc. Chemistry/Chemical Sciences; **SC** **Credits: 6**

UNIT – I

Extended Huckel Theory:

Mulliken populations, EH energies and Mulliken populations. Comparison with experimental energies. Orbital Symmetry, Building of Interaction of diagrams. Construction of Walsh diagrams and modelling potential energy surfaces. Rules for determining relative orbital energies. Conjugation and Hyperconjugation.

UNIT – II

Self Consistent Theory of molecules:

Roothan`s equations, Semi-empirical SCF methods. *Ab-initio* MO calculations. Basis sets. The Hartree-Fock limit. Correlation energy, Koopmans theorem. Perturbation theory and configuration interaction. Basis Set superposition error.

UNIT – III

Potential Energy & Surfaces:

Valence Bond configuration mixing diagrams. Rules for mixing VB configurations. VBCM and resonance theory. Reaction Profiles. Potential energy surfaces. Curve crossing Model. Factors governing barrier heights.

UNIT – IV

Molecular Mechanics:

Quantum Mechanical and Molecular Mechanics potential functions. MM force fields. Parameterization. Steric energies, Heats of formation and strain.

UNIT – V

Laboratory Sessions:

Z-matrix specification, Input for Semi-empirical and *ab-initio* programs. Molecular mechanics program. Analysis of output.

Recommended Books:

1. J.P. Lowe: Quantum Chemistry, Academic Press, New York, 1978
2. U. Burkert and N.L. Allinger: Molecular Mechanics, ACS Monograph, 1977, American Chemical Society.
3. Albright, Burdett, and Whanghbo, Approximate Molecular Orbital Theory, Academic Press, 1985
4. MOPAC 6.0 Manual and computer program, QCPE edition.
5. PCMODEL Manual and Computer program, Serena Software

CHEM 646 Advances in Nanomaterials and Photo catalysis

Pre-requisites: M.Sc Chem./Chemical Sciences; **SC** **Credits: 6**

UNIT – I

Fullerenes, Carbon nanotubes, Nanocomposites and nanofillers: formation, properties. Electronic structure. Applications. Quantum dots: Synthesis, detection and electronic structure. Metal nanoparticles and core shell nanoparticles. Monolayers: Growth process-preparation and structure, surface dynamics. Clusters in gas phase: Formation and growth, detection and analysis, types, properties and bonding

UNIT – II

Investigation and Manipulation of Nanomaterials

Instrumentation: Electron microscopies; Scanning electron microscopy, Scanning tunneling microscopy, Transmission electron microscopy, Atomic force microscopy, Small-angle X-ray scattering analysis. Optical microscopies: Confocal microscopy, Photoelectron microscopy, X-ray diffraction methods.

UNIT – III

Photocatalysis: Semiconductors, metal-

doped semiconductors, Light absorption characteristics. Interfacial electron transfer reactions,hydrogen production. Photoreaction techniques.
Applications: Molecular electronics. Biomolecular imaging. Nanomedicines: Medical diagnosis, Targeted drug delivery. Nanosensors, Molecular Nanomachines, Green in Nanoscience, Nanomaterials in environmental clean-up.

Recommended books

1. S.C. Tjong "*Nanocrystalline Materials: Their Synthesis-Structure-Property Relationships & Applications*" Elsevier Ltd, London, **2006**.
2. José A. Rodríguez, Marcos Fernández-García "*Synthesis, Properties and Applications of Oxide Nanomaterials*" John Wiley & Sons, Inc, Canada, **2007**.
3. C. Br´echignac P. Houdy M. Lahmani, *"Nanomaterials and Nanochemistry"* Springer Berlin Heidelberg, New York, **2007**.
4. Carl C. Koch, I Lya A. Ovid'ko, Sudipta Seal and Stan Veprek "*Structural Nanocrystalline Materials Fundamentals and Applications*" Cambridge University Press, Cambridge, **2007**.

CHEM 702 DISSERTATION
Pre-requisite: Consent of Teacher
HC; **Credits: 15**

Students are selected on the basis of their performance in the M. Phil entrance examination. They are allotted to various faculties of the department according to their choices and availability of position. Selected students will work independently on specialized problems related to the research interests of the respective guides. They will also submit a report on completion of the project which will be evaluated by the guide and an external examiner.

CHEM 703 *VIVA – VOCE*
Pre-requisite: CHEM 702; **HC; Credits: 3**

Students who have completed CHEM 702 will defend their work in a viva-voce in presence of examiners.