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

**CHEM 660 Chemical bonding and reactivity 4-0-2-6**

*Pre-requisite: M. Sc. Chemistry / Chemical Sciences*

***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 rectivity 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 – corelation 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 4-0-2-6**
Pre-requisite: M. Sc. Chemistry / Chemical Sciences; SC

*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 heavi 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 splittings – 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 4-0-2-6**

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

***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 excercises

***Unit II (Molecular Recognition)***

Designed Host-Guest relationships ( based on oxygen, nitrogen and aromatic macrocyles) – 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., Syntheis 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 4-0-2-6**

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

***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 enegy surfaces. Rules for determining relative orbital enrgies. 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. Parametrization. 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, Approximte 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 702 Dissertation 0-20-0-15**

*Pre-requisite: Consent of Teacher*

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 0-3-0-3**

*Pre-requisite: CHEM 702*

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