[A-3]COURSE SYLLABUS

1. Course Description (Approximately 100 words)

The goal of the course is to provide students with a fundamental understanding of the quantum chemical description of atoms and molecules. Particular emphasis is placed on the understanding of chemical bonding and reactivity, together with the theoretical basis for optical spectroscopy. The course also provides the fundamental quantum chemical background required for further courses in molecular modelling, NMR spectroscopy, inorganic chemistry and physical organic chemistry. It also deals with the applications of Quantum Mechanics to the problems of Chemistry. It begins with the fundamentals of quantum mechanics including the origin of quantum mechanics.

2. Course Goals and Objectives (Approximately 100 words)

After completing the course the students is expected to be able to:

Understand quantum chemical principles and the necessary mathematical techniques, especially the superposition principle and the variation principle.

Explain the solution of the Schrödinger equation for a particle in a box and the tunneling effect for a square barrier.

Write the electronic and total Hamiltonian operators for any molecule and explain the meaning of each part.

Use the concept of shielding (screening) to explain the properties of atoms in molecules and crystals: electronegativity, ground state of transition metals, trends in ionization energies and electronegativities, the difference in binding properties for different oxidation states, crystals.

Explain in detail the quantum chemical description of angular momentum and spin for a

3. Textbook (Title, Author, Publisher, Year of Publication, etc.)

Introduction to Quantum Chemistry 1st Edition by Clifford E. Dykstra

Quantum Chemistry 2nd Edition by Donald A. McQuarrie (Author)

4. Reference

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (Dover Books on Chemistry) Revised ed. Edition by Attila Szabo (Author), Neil S. Ostlund (Author)

5. Course Requirements and Grades

EXAM = 70%
C.A.T. = 20%
QIUZES=10%

TOTAL = 100%

6. Course Calendar

Week	Main Content
1	Introduction - chemistry as a branch of mechanics
2	linear operators - eigen function and values
3	Wave properties of EM radiation
4	photoelectric effect AND quantisation of matter
5	Matter waves:- group velocity
6	elation between group velocity and phase velocity
7	CAT AND PRESENTATIONS
8	SCHRODINGER WAVE FUNCTION
9	PARTICLE IN A BOX
10	SCHRODINGER WAVE FUNCTION
11	Angular momentum
12	Shape of orbitals
13	SUMMARY, REVISION AND ASSIGNMENTS
14	EXAMINATION