# [A-3]COURSE SYLLABUS

## 1. Course Description (Approximately 100 words)

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids.This course deals with different aspects of computational chemistry. Some fundamental computational techniques such as interpolation, matrix methods, the Newton - Raphson method, Fourier transforms and curve fitting .

## 2. Course Goals and Objectives (Approximately 100 words)

Some Challenges for Chemists and Chemical Engineers

1. Develop computer methods that will accurately predict the properties of unknown compounds.
2. Develop reliable computer methods to calculate the detailed pathways by which reactions occur in both ground states and excited states, taking full account of molecular dynamics as well as quantum and statistical mechanics.
3. Develop reliable force fields for molecular mechanics calculations on complex systems, including those with metallic elements.

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

Introductory books on quantum chemistry, statistical mechanics and computer programming fundamentals.

## 4. Reference

Introductory books on quantum chemistry, statistical mechanics and computer programming fundamentals.

## 5. Course Requirements and Grades

CAT 30%
EXAM 70%

## 6. Course Calendar

| Week | Main Content |
|---|---|
| 1 | Introduction |
| 2 | Basic Programming Techniques |
| 3 | Interpolation and Curve Fitting |
| 4 | Roots of Equations |
| 5 | Matrix Methods |
| 6 | Matrix Methods------Continued |
| 7 | MID-TERM EXAM |
| 8 | Differential Equations |
| 9 | Differential Equations--------Continued |
| 10 | Numerical Integration |
| 11 | Numerical Integration-------Continued |
| 12 | Integral Transforms |
| 13 | Integral Transforms-------Continued |
| 14 | FINAL EXAMINATION |