

# Minnesota State University Moorhead

## CHEM 460: Physical Chemistry II

### A. COURSE DESCRIPTION

Credits: 3

Lecture Hours/Week: 3

Lab Hours/Week: 0

OJT Hours/Week: \*.\*

Prerequisites:

MATH 262 - Calculus II AND CHEM 450 - Physical Chemistry I

Corequisites: CHEM 465

MnTC Goals: None

A continuation of physical chemistry 450. Topics include introduction to quantum theory, group theory, spectroscopy and statistical mechanics.

**B. COURSE EFFECTIVE DATES:** 05/19/1999 - Present

### C. OUTLINE OF MAJOR CONTENT AREAS

1. Kinetic Theory of Gases
2. Using Quantum Mechanics on Simple Systems
3. The Particle in The Box and the Real World
4. Commuting and Noncommuting Operators
5. A Quantum Mechanical Model: Vibration and Rotation of Molecules
6. The H atom
7. Many-Electron Atoms
8. The Chemical Bond in Diatomic Molecules
9. Molecular Symmetry
10. Elementary Chemical Kinetics
11. Complex Reaction Mechanisms
12. From Classical to Quantum Mechanics, Quantum Chemistry
13. The Schrodinger Equation
14. The Quantum Mechanical Postulates

#### **D. LEARNING OUTCOMES (General)**

1. Use the quantum mechanical postulates to calculate observable values of quantum mechanical systems.
2. Apply quantum mechanical postulates to simple systems starting with the particle in a one-dimensional box in an infinite potential well.
3. Calculate the energy and wave functions the one-dimensional box with finite potential barriers. Use the model to explain covalent bonding, metallic bonding, tunneling through potential barriers and tunneling in chemical reactions.
4. Define terms to describe reaction rates, derivation of reaction rate laws and integration of rate law expressions. Explain reversibility and equilibrium states of chemical reactions. Explain reaction rate theories and construct potential energy surfaces for chemical reactions.
5. Derive the equation of state based on Kinetic theory. Use the Maxwell distribution of molecular speeds to describe ensembles of molecules. Derive the expressions for molecular collisional rates and mean free paths.
6. Explain the reason and the experiments that lead to the need for studying quantum mechanics.
7. Formulate the Schrödinger equation and solve the Schrödinger equation for the Hydrogen atom. Interpret eigenvalues and eigenfunctions from the solution of Schrödinger equation and model the hydrogen atom.
8. Formulate the Schrödinger equation for many-electron atoms. Explain the reason that lead to the requirement of the spin function in the total wave function. Construct wavefunctions that include the property of indistinguishability of electrons in multi-electron systems. Use the Variation method to solve the Schrodinger equation and Hartree-Fock self-consistent field calculations. Appreciate the basis of quantum numbers electrons in atoms.
9. Identify the systems that are describable by Quantum mechanics. Explain the features of the Schrödinger equation. Construct operators relevant to solve the eigenequation. Interpret eigenvalues and eigenfunctions.
10. Propose and explain complex reaction mechanisms. Explain and use pre-equilibrium approximation and the Lindemann mechanisms in reaction kinetics mechanisms. Explain the concept of catalysis.
11. Set up calculations in advanced molecular modeling software with graphical inputs and outputs. Perform calculations at Hartree-Fock level and beyond of molecular geometries, thermodynamic properties, kinetics of reactions and IR, UV, NMR spectra of model compounds.
12. Solve the Schrödinger equation for many electron molecules. Express the molecular orbitals as a linear combination of atomic orbitals. Construct molecular orbital diagrams for diatomic molecules. Interpret molecular parameters bond order, bond energy, and bond length.
13. Use and interpret commuting and non-commuting operators in quantum mechanics. Explain the Heisenberg uncertainty principle.
14. Use the quantum mechanical model to calculate the vibration and rotation energies and wavefunctions of molecule, eventually explain and extract molecular parameters such as molecular geometries and bond energies from molecular spectra.

#### **E. Minnesota Transfer Curriculum Goal Area(s) and Competencies**

None

#### **F. LEARNER OUTCOMES ASSESSMENT**

As noted on course syllabus

#### **G. SPECIAL INFORMATION**

None noted