# Chemistry 3140 Physical Chemistry II
# Spring 2022

**Instructor:** Kevin Morris, DSC 178
**Office Hours:** T 10-12, R 1-3, F 9-10 and by appointment either in-person or on Zoom.
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## Textbook

Peter Atkins and Julio de Paula: *Physical Chemistry, 11th Edition*

## Course Plan

CHM 3140 completes a yearlong introduction to physical chemistry. We will begin with the historical development of quantum mechanics, followed by an introduction to the basic principles of quantum theory and operator formalism. Translational, vibrational, and rotational motion and angular momentum will then be analyzed using the particle-in-a-box, harmonic oscillator, and particle-on-a-sphere models, respectively. This background will allow us to understand atomic and molecular structure, beginning with hydrogen-like atoms and proceeding through chemical bonds. Finally, our discussion of molecular spectroscopy will be divided into rotational/vibrational and Raman spectroscopy, electronic spectroscopy, NMR spectroscopy, and lasers. We will also discuss molecular modeling and computational chemistry topics.

## Homework and Exams

Physical chemistry is a quantitative subject and solving problems is the best way to learn the material. Problem assignments will be made on Monday of each week and collected the following Monday. The problem sets will include a selection of problems from the end of each chapter in the textbook and supplemental problems that involve more complex calculations or graphical analyses.

We will also have three exams and a comprehensive final. Exams I and II will contain both in-class and take-home sections. The take-home questions will be distributed the class period before the exam and collected at the beginning of the exam period. Exam III will be a take-home test. The final is comprehensive over the semester. All exams should be taken during the scheduled time unless prior arrangements are made. Exam dates are given below.

Exam I: Wednesday, March 9th
Exam II: Wednesday, April 13th
Exam III: Take-Home Exam is due Wednesday, May 11th

## Writing Assignments

We will also have two writing assignments this semester. In the 20th century, many physicists and physical chemists won Nobel Prizes for developing the new theory of quantum mechanics and applying it to atoms, molecules, and spectroscopy. These scientists include familiar names like Max Plank, Albert Einstein, Marie Curie, Irene Joliot-Curie, Niels Bohr, Louis de Broglie, Werner Heisenberg, Erwin Schrodinger, Wolfgang Pauli, Ernest Rutherford, Peter Debye, Maria Mayer, Linus Pauling, and Dorothy Hodgkin. In our first writing assignment, everyone will pick a Nobel Prize-winning scientist from the early 20th century and write a short paper (4 to 5 pages) describing his or her work. The paper should be non-technical and accessible to someone who has taken General Chemistry and Physics.

Deadlines for Nobel Prize paper are given below.

Friday, February 18st: Turn in the paper topic and a draft outline.
Friday, March 4th: Turn in a draft of the paper
Friday, March 25th: Turn in final paper

In the second assignment, we will assign and analyze the high-resolution IR spectrum of HCl vapor. We will also calculate the molecule's force constant, rotational constant, and moment of inertia. Unlike the first assignment, this report will involve analyzing spectra, graphing data, and performing calculations. The HCl report is due Friday, May 6th.

## Spartan

We will use the Spartan molecular modeling program in a number of assignment this semester. We have a site license that allows students and faculty to download the software onto their computers. Spartan will then run as long as you are connected to the Carthage network. Directions for downloading and installing Spartan are on Schoology.

## Grades

The final grade will be computed as follows.

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|---|---|
| **Exams and Final** | **50%** |
| **Homework Problems** | **30%** |
| **Papers** | **20%** |

## Students with Disabilities

Carthage College strives to make all learning experiences as accessible as possible. If you anticipate or experience academic barriers due to a disability (including mental health, learning disorders and chronic medical conditions), please notify the instructor so we can privately discuss options. To establish reasonable accommodations, also register with Diane Schowalter in Learning Accessibility Services (dschowalter1@carthage.edu).

## Personal Protective Equipment

Carthage's policies regarding face masks and social distancing can be found at https://www.carthage.edu/life-at-carthage/health-wellness-safety/covid-19/. Please read and comply with all listed policies and rules.

## Academic Honesty

Students are expected to adhere to the College's code of academic conduct found at www.carthage.edu/current-students/community-code/student-conduct-system/. Academic misconduct includes copying, plagiarizing, duplicating, or misrepresenting work by others on exams, papers, and assignments. This includes material found on Chegg and other homework cheat sites. Academic dishonesty will be handled by assigning a grade of zero on the affected work for the first offence, and failure of the course on subsequent offences.

## Lecture Schedule

| Week of | Topics | Text Chapter |
|---|---|---|
| **February 2** | Black Body Radiation and the Photoelectric Effect<br>Hydrogen Atom Spectrum | 7 |
| **February 7** | Postulates of Quantum Mechanics<br>Schrodinger's Equation | 7, 8 |
| **February 14** | Particle in a One, Two and Three Dimensional Box<br>Tunnel Effect<br>*Turn in Nobel Prize paper topic and outline* | 8 |
| **February 21** | Vibrational Motion and the Harmonic Oscillator<br>Rotational Motion and Angular Momentum | 8, 9 |
| **February 28** | Hydrogen Atom<br>*Turn in first draft of Nobel Prize Paper* | 9 |
| **March 7** | Electron Spin and Many-Electron Atoms<br>**Exam I** | 10 |
| **March 21** | Born-Oppenheimer Approximation<br>Valence Bond and Molecular Orbital Theory<br>*Turn in final draft of Nobel Prize Paper* | 10 |
| **March 28** | Huckel Theory and Aromatic Molecules<br>Molecular Modeling Calculations | 10 |
| **April 4** | Introduction to Molecular Spectroscopy<br>Molecular Rotations and Microwave Spectroscopy | 12 |

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|---|---|---|
| **April 11** | IR spectroscopy of Diatomic Molecules<br>**Exam II** | |
| **April 18** | Complete IR Spectroscopy<br>Raman Spectroscopy | 12 |
| **April 25** | Electronic Transitions and Optical Spectroscopy<br>Lasers | 13 |
| **May 2** | Nuclear Spin and NMR Spectroscopy<br>Pulse Sequences and Spin Echoes<br>*Turn in HCl paper* | 14 |
| **May 9** | Nuclear Overhauser Effect<br>Fourier Transforms<br>**Take-Home Exam** | 14 |
| **May 16** | Final Exam | |

**Learning Objectives**

1. To understand how experiments from the early 20th century lead to the development of quantum theory.

2. To be able to write Schrodinger's equation for a particle in a box, harmonic oscillator, particle on a sphere and simple atoms and molecules.

3. To understand and apply the postulates of quantum mechanics.

4. To be able to apply the principles of quantum mechanics to the hydrogen atom and associate hydrogen atom wavefunctions with atomic orbitals.

5. To be able to apply the principles of quantum mechanics to atoms with more than one electron and write term symbols for electron configurations.

6. To understand quantum mechanical approximation methods like the variational theorem.

7. To understand the Born-Oppenheimer approximation and molecular orbital theory and to be able to use them to describe the bonding in diatomic and conjugated organic molecules.

8. To understand how modeling techniques like *ab initio* calculations, molecular mechanics, density functional theory, and molecular dynamics are used to study chemical systems.

9. To be able to predict if a molecule or a vibrational normal mode is microwave/IR active and to understand the rotational fine structure of high-resolution IR spectra.

10. To understand the physical principles underlying Raman spectroscopy and to be able to predict if a vibrational mode is Raman active.

11. To understand the physical principles underlying electronic absorption spectroscopy, lasers, fluorescence, and phosphorescence.

12. To understand the concept of nuclear spin, the operation of a pulsed NMR spectrometer and to be able to describe how rf pulses are used to generate spin echoes and two-dimensional NMR spectra.