

**Chem 3620, Physical Chemistry II, Winter 2002**

Class Times: TTh 10:00 – 11:50 am, Olin 103

Instructor: Sandra S. Eaton

Office: Seeley G. Mudd Rm. 178

Office Hours: T Th 8-10 am, or by appointment

**Text:** *Physical Chemistry*, P. Atkins and J. de Paula, 7th ed., Freeman, 2002.**Course Outline (Updated 3/03/02)**

| Date   | Topic   | Reading in Atkins and de Paula | Homework - E and P refer to Exercises and Problems from Atkins and de Paula |
|--------|---|--------------------------------|---|
| Jan. 3 | Problems with Classical Mechanics                         | p. 293-304                     |   |
| 8      | Uncertainty Principle, Wave Packets                       | 317-320                        |   |
| 10     | Schrödinger Equation, Expectation Values                  | 304-317                        | 9.1, 9.3, 9.5, 9.9, 9.10 (from Silbey and Alberty)                          |
| 15     | Particle in 1-D box                                       | 325-331                        |   |
| 17     | 3-D box, box with sloping bottom                          | 331-334                        | P11.5, P11.16, P11.20, E12.5b, E12.7b                                       |
| 22     | Harmonic Oscillator                                       | 338-345                        |   |
| 24     | Rotational Motion   | 345-352                        | E12.9b, E12.10b, E12.12b, E12.15b, P12.27                                   |
| 29     | Exam 1  |                                |   |
| 31     | Hydrogen Atom   | 365-372                        | E12.17b, E12.18b, P12.4   |
| Feb. 5 | Hydrogen-like Wavefunctions                               | 372-383                        |   |
| 7      | Electron Spin   | 352-355                        | E13.5b, E13.6b, E13.10b, E13.16b, P13.2                                     |
| 12     | Multielectron Atoms                                       | 383-392                        |   |
| 14     | H <sub>2</sub> Molecule                                   | 410-422                        | E13.14b (note: $R_H = R_{atom}$ ), E13.19b, P13.12, P13.21, P13.26b         |
| 19     | Diatomic Molecules  | 422-432                        |   |
| 21     | Exam 2  |                                | E14.5b, E14.7b, E14.9b, P14.5, P14.7  |
| 26     | Symmetry, Point Groups                                    | 453-462                        |   |
| 28     | Character Tables, Molecular Orbitals for H <sub>2</sub> O | 463-471                        |   |
| Mar. 5 | Rotation Spectra  | 481-490, 497-501               | E15.7b (change $D_{6h}$ to $D_{3h}$ ), E15.13b, E15.14b, E15.15b, E15.16b   |
| 7      | Vibrational Spectra                                       | 511-515, 517-523               |   |
| 12     | Review/overview   |                                | E16.8b, E16.11b, E16.18b, E16.19b, P16.5                                    |
| 14     | Final exam – cumulative                                   |                                |   |

Grading: Class Participation - 10%, Homework - 15%, Exams - 25% each.

## Physical Chemistry II Winter 2001

| <b><i>CHEMICAL KINETICS</i></b>                  |  |
|--|--|
| Tues Jan 2                                       | Session 1: The microscopic view of matter. Maxwell distributions of velocities and speeds. Transport properties. (Chapter 3)   |
| Thurs Jan 4                                      | Session 2: Kinetics of elementary reactions. (Chapter 12, sections 1-3)  |
| Tues Jan 9                                       | Session 3: Reaction mechanisms; reversible and consecutive reactions and the steady-state approximation. (Chapter 12, section 4).  |
| Thurs Jan 11                                     | Session 4: Theories of reaction rates; potential energy surfaces and transition state theory. Effect of temperature and isotopic exchange on the rate constant. (Chapter 12, sections 5-8) |
| Tues Jan 16                                      | <b>Discussion and review</b>   |
| Thurs Jan 18                                     | <b>Exam # 1</b>  |
| <b><i>INTRODUCTION TO QUANTUM MECHANICS</i></b>  |  |
| Tues Jan 23                                      | Session 5: Failure of Classical Physics: Planck, Einstein, and Bohr. (Chapter 14, sections 1-4).   |
| Thurs Jan 25                                     | Session 6: The wave particle duality and wave packets. (Chapter 14, sections 5-6 and supplementary material).  |
| Tues Jan 30                                      | Session 7: The Schrodinger equation and applications to one dimensional systems. (Chapter 14, sections 7-9).   |
| Thurs Feb 1                                      | Session 8: One dimensional systems, continued.   |
| Tues Feb 6                                       | Session 9: Determination of physical properties from mathematical wave functions. Eigenvalues and expectation values. (Supplementary material)   |
| Thurs Feb 8                                      | Session 10: Eigenvalues and expectation values, continued.   |
| Tues Feb 13                                      | <b>Discussion and review</b>   |
| Thurs Feb 15                                     | <b>Exam #2</b>   |
| <b><i>QUANTUM MECHANICS AND SPECTROSCOPY</i></b> |  |
| Tues Feb 20                                      | Session 11: The harmonic oscillator and vibrational motion. (Supplementary material).  |
| Thurs Feb 22                                     | Session 12: Rotational Motion and the flooded planet. (Supplementary material).  |
| Tues Feb 27                                      | Session 13: Microwave and infrared spectroscopy (Chapter 17, sections 2-3).  |
| Thurs Mar 1                                      | Session 14: The hydrogen atom. (Chapter 14, sections 10-11).   |
| Tues Mar 6                                       | Session 15: The hydrogen atom, continued.  |
| Thurs Mar 8                                      | <b>Discussion and review</b>   |
|  | <b>Final Exam (at 10:00 am)</b>  |

## COURSE INFORMATION

Credit hours: 3 quarter hours

Time: 10:00-11:50 am, Tuesday and Thursday

| Grading:       |     |
|----------------|-----|
| Worksheets     | 45% |
| Two hour exams | 30% |
| Final exam     | 25% |

This course will be somewhat different from the usual lecture style course. It has been divided into 15 sessions as listed on the course syllabus. The majority of your time in each session will be spent working on worksheets that will take you through the material to be covered that day. The worksheets, which are due at the beginning of the next session, include problems from the textbook. For some sessions there will be a short introduction. Before each exam, there will be a review session.

This course is structured to take advantage of the fact that learning takes place when one is actively engaged in the process. The time spent in this class will be characterized by active student participation in the completion of worksheets, which will be available through this course website. Before coming to class, you will be expected to read the sections noted at the beginning of the worksheet, download the worksheet and bring it to class. You are encouraged to work on the worksheets before class, but you will find that it will be necessary to attend class to gain a thorough understanding of the material.

When you graduate from DU your education will not stop. Whether you get a job or go on to a graduate or professional school, you will be expected to continue to learn new information often without the benefit of a formal instructor who will tell you what to learn. The structure of this course should help you make this transition and help you to become an independent learner.