

Chemistry 1410: Physical Chemistry 1

Spring 2009 – 3 Credits

Course Information and Syllabus

Instructor: Sunil K. Saxena, 711 Chevron Science Center
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Course Hours and Location: Tue, Thu 11:00 am - 12:15 pm, Chevron 12B

Recitations: Tue 3:00 pm - 3:50 pm, Chevron 12B

Text:

“Quantum Chemistry and Spectroscopy”, Thomas Engle

Course Goals: To introduce you to quantum mechanics so as to quantitatively discuss chemical bonding and spectroscopy.

Office Hours: Mon 10:00-11:30 and Thu 2:00-3:30

Course Grading: In class examinations, home work assignments.

Grades Distribution:

Exam 1: 25 % *Exam 2: 25 %* *Exam 3: 30 %*
Assignments: 20 %

Exams: There will be three in-class exams during the semester. The first exam will be on **Thursday February 5th** and the second on **Thursday March 5th**. Each will be about 75 minutes long. The final exam is scheduled for **Tuesday April 21st at 8:00 – 9:50 am**. Each exam will focus on material covered after the preceding exam (the third exam is not cumulative). More details on coverage for each exam will be outlined in class at least a week before the exam. You will be allowed to bring in a 8.5×11 inch sheet of paper with fundamental constants, parameters, and any key equations or material that you will feel will help in the exam. No make-up exams will be given. If you miss an exam you will be assigned a score of zero. If the failure to take an exam is due to a serious illness or extreme emergency (documentation is required) then the other two exams will be averaged to decide your score.

Assignments: To aid the study of class material you will be given regular assignments (roughly one every two weeks). You will find that a thorough understanding of each problem set will help you master concepts. The assignments will be graded.

Syllabus

Particles, waves, the Schrodinger's equation, postulates of quantum mechanics, models of molecular motion, chemical bonding, vibrational and rotational spectroscopy, molecular spectroscopy, magnetic resonance spectroscopy.

Course Schedule

Note: The schedule of lectures is tentative, although every effort will be made to stay on schedule.

Jan 6 (T)	8 (Th)
<p><i>Lecture 1</i> - Syllabus - Introduction, Classical mechanics reviewed</p>	<p><i>Lecture 2</i> - black body radiation, photoelectric effect, atomic spectra are discrete lines, electrons diffract like light (Chapter 1)</p>
13 (T)	15 (Th)
<p><i>Lecture 3</i> - how light behaves, some math, adapting equations for light to matter (Chapter 2) (HW 1 assigned)</p>	<p><i>Lecture 4</i> - Schrodinger's Equations and postulates of QM (Chapter 3)</p>
20 (T)	22 (Th)
<p><i>Lecture 5</i> - Particle in free space, box (Chapter 4) (HW 2 assigned)</p>	<p><i>Lecture 6</i> - particle in a box, examples and use of postulates (Chapter 4)</p>
27 (T)	29 (Th)
<p><i>Lecture 7</i> - Particle in a finite box,</p>	<p><i>Lecture 8</i> - PIB Models in Physical Chemistry, Particle in a Cube</p>
Feb 3 (T)	5 (Th)
<p><i>Lecture 9</i> - Heisenberg Uncertainty</p>	- Exam 1
10 (T)	12 (Th)
<p><i>Lecture 10</i> - vibrational motion</p>	<p><i>Lecture 11</i> - rotational motion in 2D</p>
17 (T)	19 (Th)
<p><i>Lecture 12</i> - rotational motion in 3D</p>	<p><i>Lecture 13</i> - vibrational spectroscopy</p>

Feb 24 (T)	26 (Th)
<i>Lecture 14</i> - vibrational spectroscopy	<i>Lecture 15</i> - rotational effects, IR, Raman, Gas phase spectra
Mar 3 (T)	5 (Th)
- the Hydrogen atom	<i>Lecture 16</i> - Exam 2
17 (T)	19 (Th)
<i>Lecture 17</i> - the Hydrogen atom, Spin (NO CLASS)	<i>Lecture 18</i> - He, and one electron orbitals
24 (T)	26 (Th)
<i>Lecture 19</i> - Slater Determinants, Hartree Fock Self Consistent Field Approach	<i>Lecture 20</i> - Total Angular Momentum, Energy and Term Symbols
31 (T)	Apr 2 (Th)
<i>Lecture 21</i> - Chemical Bonding	<i>Lecture 22</i> - Chemical bonding
7 (T)	9 (Th)
<i>Lecture 23</i> - Chemical bonding	<i>Lecture 24</i> - Chemical Bonding
14 (T)	16 (Th)
<i>Lecture 25</i> - Electronic Spectroscopy	<i>Lecture 26</i> - magnetic resonance
21 (T)	
- Exam 3 (8:00-9:50 am)	