Chem 3630, Physical Chemistry III, Spring 2008
Schedule

Date	Topic	Reading
Part 1: Introduction to Quantum Mechanics		
3/25	Worksheet #1: A brief look at classical mechanics.	Appendix 3
3/27	Worksheet #2: The advent of quantum mechanics.	1.1 – 1.2
4/1	Worksheet #3: The Basics of quantum mechanics: the Schrodinger equation, operators, observables, eigenfunctions & eigenvalues	1.3 – 1.6 Properties of the wavefunction
4/3	Worksheet #4: Using the Schrodinger equation: the free particle and the particle in a box equation	2.1-2.3
4/8	Presentations by students **REVIEW**	Applications
4/10	**EXAM #1**	
Part 2: Quantum Mechanical Models for Atoms & Molecules		
4/15	Worksheet #5: Using the Schrodinger equation: harmonic oscillators and rigid rotors (models for molecular motion)	2.4 – 2.7
4/17	Worksheet #6: Vibrational/rotational spectroscopy	6.1 – 6.7
4/22	Worksheet #6 continued	6.9 – 6.13
4/24	Worksheet #7: The hydrogen atom	3.1 – 3.3
4/29	Worksheet #8: Many electron atoms & an introduction to approximation methods	3.4 and the section on "Hartree-Fock Algorithm" found at http://en.wikipedia.org/wiki/Hartree-Fock_method
5/1	Presentations by students **REVIEW**	Applications
5/6	**EXAM #2**	
Part 3: Approximation Methods for Real Systems		
5/8	Finish Part IV of Worksheet #8: an introduction to approximation methods Worksheet #9: Structure & Spectra of Many-electron Atoms	3.4 – 3.9
5/13	Worksheet #10: Molecular structure: diatomics	4.1 – 4.5
5/15	Worksheet #11: Molecular structure: polyatomics	4.3 – 4.5
5/20	Worksheet #12: Polyatomic molecules	4.6 – 4.8
5/22	Group projects - computations with Gaussian	Handout
5/27	Group projects - computations with Gaussian	
5/29	Presentations by students **REVIEW**	Applications
6/3	**EXAM #3 (9 – 11 am)**	