

Chem 321 Assignment Schedule

Prof. Adam Van Wynsberghe

Fall 2014

Week	Date	Lecture Topic	Reading	Laboratory	Assignments
1	8/29 F	Class Introduction		No Lab	
2	9/1 M	Classical Failures; Rydberg Formula; de Broglie	1.1-7	Intro to P-chem Lab	
	9/3 W	Bohr Model and Heisenberg's Uncertainty Principle	1.8-9; Math Chapter A		
	9/5 F	Double-Slit Experiment Classical Wave Equation	2.1-5		HW #1
3	9/8 M	Classical Wave Equation	2.1-5; Math Chapter B	Intro to Computational Modeling	
	9/10 W	Schrödinger Equation; Operators	3.1-4		
	9/12 F	Particle in a Box	3.5-6		HW #2
4	9/15 M	Particle in a Box	3.7-8; Math Chapter C		
	9/17 W	Particle in a 3-D Box	3.9		
	9/19 F	Postulates of Quantum Mechanics	4.1-3		HW #3
5	9/22 M	Postulates of Quantum Mechanics	4.4-6	Magnetic Susceptibility and Cryoscopy	
	9/24 W	EPR and Bell's Inequality			
*** Exam I: Due Friday, September 26th, 11:00 AM ***					
	9/26 F	Classical Harmonic Oscillator	5.1-3		

6	9/29 M	QM HO; Spherical Coordinates	5.4-7; Math Chapter D	
	10/1 W	Rigid Rotator	5.8-9	
	10/3 F	Molecular Interactions with Light	13.11	HW #4
7	10/6 M	Vibrational Selection Rules	13.12	FT-IR Spectra of HCl and DCl
	10/8 W	Rotational Selection Rules; Ro-vib spectra	13.13; 13.1-2	
	10/10 F	Deviations from HO/RR; Vibronic spectra	13.3-7	HW #5
8	10/13 M	Hydrogen Atom–Angular Equation	6.1-6.2	
	10/15 W	Hydrogen Atom–Angular Momentum and Radial Equation	6.3-6.4	
	10/17 F	No Lecture-Fall Recess		
9	10/20 M	Hydrogen Atom–Orbitals	6.5-6.7	UV-vis Spectroscopy of TM Complexes and Aromatics
	10/22 W	Variational Theory	7.1; Math Chapter E	HW #6
*** Exam II: Due Friday, October 24th, 11:00 AM ***				
	10/24 F	Secular Equation	7.2-3	

10	10/27 M	Perturbation Theory; Atomic Units	7.4; 8.1	
	10/29 W	Hartree-Fock; Stern-Gerlach	8.2-3	
	10/31 F	Spin; Slater Determinants	8.4-6	HW #7
11	11/3 M	Term Symbols	8.8-9	Fluorescence, Luminescence and Thermochromism
	11/5 W	Hund's Rules; Atomic Spectra	8.10-8.11	
	11/7 F	Born-Oppenheimer Approximation	9.1-4	HW #8
12	11/10 M	Diatomic Bonding; Molecular Orbitals of Diatomics	9.5-11	
	11/12 W	Heteronuclear Diatomics	9.12-13	
	11/14 F	Molecular Term Symbols	9.14-16	HW #9
13	11/17 M	Molecular Shapes	10.1-4	Advanced NMR techniques
	11/19 W	Valence Bond; Polyatomic MO	10.1-2	
*** Exam III: Due Friday, November 21st, 11:00 AM ***				
	11/21 F	Walsh Correlation Diagrams	10.3-4	
Thanksgiving Break!				

14	12/1 M	Hückel Theory	10.5-7	X-ray Diffraction Methods	
	12/3 W	Practical Hartree-Fock	11.1		
	12/5 F	Gaussian Type Functions	11.2-4		HW #10
15	12/8 M	Gaussian Basis Sets		Oral Presentations	
	12/10 W	Post Hartree-Fock <i>ab initio</i> electronic structure			
	12/12 F	Density Functional Theory			

***** Final Exam: Due Thursday, December 18th, 10:00 PM TSC 1004 *****
