

Course Outline

Week	Date (* indicate HW due)	Lecture	Text
Fundamentals of Quantum Mechanics			
1	Jan. 23 (Mon) Jan. 25 (Wed) Jan. 27 (Fri)* ¹	Origins of quantum mechanics Classical Mechanics (harmonic oscillator) Schrödinger equation, operators	Chapt. 7
2	Jan. 30 (Mon) Feb. 1 (Wed) Feb. 3 (Fri)* ²	Observables and expectation values Uncertainty principle Particle in a box	Chapt. 8
3	Feb. 6 (Mon) Feb. 8 (Wed) Feb. 10 (Fri)* ³	2-D particle in a box, degeneracy, tunneling Vibrations, harmonic oscillator Particle on a ring and angular momentum	
4	Feb. 13 (Mon)	Particle on a sphere and angular momentum	
Rotational and Vibrational Spectroscopy			
5	Feb. 15 (Wed) Feb. 17 (Fri)* ⁴ Feb. 20 (Mon) Feb. 22 (Wed) Feb. 24 (Fri)* ⁵	Spectroscopy, rotations of molecules Rotational selection rules Rotational spectra, vibrations of diatomic molecules Vibrational, rotational spectra of diatomic molecules Vibrations of polyatomic molecules	Chapt. 12
Quantum Mechanics of Atoms			
6	Feb. 27 (Mon) Feb. 28 (Tue) Feb. 29 (Wed)	Hydrogen atom Exam 1 – 7:15 pm – Room 1361 Chem No Class	Chapt. 9
7	Mar. 2 (Fri) Mar. 5 (Mon) Mar. 7 (Wed)* ⁶ Mar. 9 (Fri)	Hydrogen atom wavefunctions and spectra Multielectron atoms Aufbau, Pauli principle Singlets and triplets, perturbation calculation	
8			
Chemical Bonds (Molecules)			
9	Mar. 12 (Mon) Mar. 14 (Wed)* ⁷ Mar. 16 (Fri) Mar. 19 (Mon) Mar. 21 (Wed)* ⁸ Mar. 23 (Fri)	Born-Oppenheimer approx, valence bond theory Molecular orbital theory Diatomic molecules Diatomic molecules Heteronuclear diatomic molecules Polyatomic molecules	Chapt. 10
10			
Electronic Spectroscopy			
11	Mar. 26 (Mon) Mar. 28 (Wed)* ⁹ Mar. 29 (Thu) Mar. 30 (Fri) Apr. 2-6	Excited states, Fluorescence, Fates of excited states Review lecture Exam 2 – 7:15 pm – Room 1361 Chem No Class Spring Break	Chapt. 13
Statistical Thermodynamics			
12	Apr. 9 (Mon) Apr. 11 (Wed) Apr. 13 (Fri) Apr. 16 (Mon)	Counting, statistics, Boltzmann distribution Partition functions Translations Energy and Entropy	Chapt. 15
13	Apr. 18 (Wed) Apr. 20 (Fri) Apr. 23 (Mon) Apr. 25 (Wed)* ¹⁰ Apr. 27 (Fri)	Canonical partition function Thermodynamic functions Molecular energies Heat capacities revisited !! Equilibrium	Chapt. 16
Molecular Reaction Dynamics			
15	Apr. 30 (Mon) May 2 (Wed)* ¹¹ May 4 (Fri) May 7 (Mon) May 9 (Wed)* ¹² May 11 (Fri)	Collision theory, rate constants Diffusion controlled reactions Potential energy surfaces, Activated complex theory Activated complex theory Thermodynamic formulation Review Lecture	Handouts
16	May 15 (Tue)	Final Exam – 2:45 pm – Room TBA	