

CHM 102A part 2: Physical Chemistry: Quantum theory, structure, bonding and spectroscopy

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Lectures: T F 800, T201

Tutorials: Th 800 T201

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Course description: Quantum Theory, Quantum Mechanics of simple systems, Particle in a box, harmonic oscillator, rigid rotor, hydrogen atom, many electron atoms, Molecular orbital theory of diatomic molecules, Rotational, Vibrational and Raman spectroscopy, electronic spectroscopy

Detailed lecture-wise plan

1. **Lecture 1:** Need for a quantum theory, wave-particle duality, uncertainty principle, postulates of quantum mechanics, wavefunctions, operators, eigenvalues and eigenfunctions.
2. **Tutorial 1:** Operators, eigenvalues, eigenfunctions, expectation values, conditions on the wavefunction.
3. **Lecture 2:** Hamiltonian operator, Particle in a 1D Box, solutions, quantization.
4. **Lecture 3:** Particle in a 2D box, degeneracy
5. **Tutorial 2:** Boundary conditions in particle in a 1D box, method of separation of variables, degeneracy, most probable position, expectation values.
6. **Lecture 4:** Harmonic Oscillator model, properties of solutions, boundary conditions at infinity. Molecular bonding and Morse oscillator.
7. **Lecture 5:** 1D/3D Rigid Rotor
8. **Tutorial 3:** Expectation values in Harmonic oscillator, probabilities, tunneling, Angular momentum eigenfunctions, plotting angular momentum functions
9. **Lecture 6:** Hydrogen Atom, atomic orbitals, Radial distribution
10. **Lecture 7:** Helium Atom, Electron spin
11. **Tutorial 4:** Hydrogen atom wavefunctions, expectation values, QUIZ
12. **Lecture 8:** Molecular Orbital theory for Hydrogen molecule ion
13. **Tutorial 5:** Hydrogen atom

14. **Lecture 9:** MO theory for diatomic molecules
15. **Lecture 10:** Fundamentals of molecular spectroscopy, microwave spectroscopy
16. **Tutorial 6:** Molecular Orbital theory, Rotational spectroscopy
17. **Lecture 11:** IR spectroscopy, Raman spectroscopy
18. **Lecture 12:** Raman spectroscopy, UV-Vis spectroscopy
19. **Lecture 13:** Spectroscopy tutorial, Course evaluation

Course Highlights: This course will help you answer three questions:

1. What makes keeps the electron and the proton apart in the Hydrogen atom ?
2. What keeps two neutral Hydrogen atoms close to each other in the Hydrogen molecule ?
3. How can you see the motion of atoms in a molecule ?

Books: Text Book: Atkins' Physical Chemistry(8th Edition), by Peter Atkins and Julio De Paula: Relevant sections in Chapters 8, 9, 10, 11, 13 and 14.

Other Reference books that you might like

1. Physical Chemistry, A molecular approach, by D.A. McQuarrie and J.D. Simon
2. Physical Chemistry, by I.N. Levine

Internet Resources: There are many online resources, but there is no guarantee that they provide the correct information. I often prepare my notes after reading someone's notes on the internet. Some resources that might be useful are given below.

1. <http://ocw.mit.edu/>: MIT Open Course ware.
2. http://202.141.40.218/wiki/index.php/Introductory_Quantum_mechanics: Prof Mangala Sundar's course on Quantum Chemistry.

Grading System

1. Attendance : (5 points total)
2. Quiz : (10 points): 35 minutes hour exam to be held
3. Final Exam : (35 points): 2 hour exam.