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
Tutor: Pankaj Yadav
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


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.


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.


**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.