August 2017

Chemistry 1480: *Intermediate Physical Chemistry*

This course will survey two fundamental components of Physical Chemistry, namely: I) Quantum Mechanics and II) Statistical Mechanics.

Instructor: Rob Coalson

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Lectures: Monday, Wednesday 4:00 – 5:15 p.m.; 154 Chevron Science Center

Required Textbook: *Molecular Physical Chemistry for Engineers*, J.T Yates, Jr., and J. Karl Johnson [University Science Books, 2007; ISBN 10: 1-891389-27-0].

Teaching Assistant: Simon Wei, email: jiw105@pitt.edu

Grading: Two hourlies (25%+25%), final exam (35%), homework (15%).

Office Hours: i) Rob Coalson, 321 Eberly Hall, 1-2 pm Tuesdays
ii) Simon Wei, Chevron G-03, 1:30-2:30pm Thursdays

Mathcad: The course will make occasional use of the electronic notebook software Mathcad. This program is available in the Dept. of Chemistry's Joint Computation Center (JCC), and in all Pitt computer labs. Or, for a small fee, a single-user license can be obtained by Pitt students.

Tentative Syllabus:

Part I: Quantum Mechanics

Aug. 28 Introduction and Principles (Ch. 2).

Aug. 30 Introduction and Principles (Ch 2)

Sept. 6 Introduction and Principles (Ch. 3)

Sept. 11 Introduction and Principles (Ch. 3)

Sept. 13 Techniques and Applications (Ch. 3)

Sept. 18 Techniques and Applications (Ch. 3)

Sept. 20 Techniques and Application (Ch. 3)

Sept. 25 Atomic and Molecular Structure (Ch. 4)

Sept. 27 **1st Hour Exam**

Oct. 2 Atomic and Molecular Structure (Ch. 4)

Oct. 4 Atomic and Molecular Structure (Ch. 4)

Oct. 10 Molecular Spectroscopy (Ch. 4)

Oct. 11 Molecular Spectroscopy (Ch. 4)

Oct. 16 Molecular Spectroscopy (Ch. 4)

Oct. 18 Molecular Spectroscopy (Ch. 4)

Part II: Statistical Mechanics

Oct. 23 Basic Concepts of Statistical Mechanics (Ch. 5)

Oct. 25 Basic Concepts of Statistical Mechanics (Ch. 5)

Oct. 30 Basic Concepts of Statistical Mechanics (Ch. 5)

Nov. 1 **2nd Hr. Exam**

Nov. 6 Basic Concepts of Statistical Mechanics (Ch. 5)

Nov. 8 Computational Machinery of Statistical Mechanics (Ch. 5)

Nov. 13 Computational Machinery of Statistical Mechanics (Ch. 5)

Nov. 15 Computational Machinery of Statistical Mechanics (Ch. 5)

Nov. 20 Applications of Stat. Mech. to Molecular Thermodynamics (Ch. 5)

Nov. 27 Applications of Stat. Mech. to Molecular Thermodynamics (Ch. 5)

Nov. 29 Applications of Stat. Mech. to Molecular Thermodynamics (Ch. 5)

Dec. 4 Applications of Stat. Mech. to Molecular Thermodynamics (Ch. 5)

Dec. 6 Special Topics

Week of Dec. 11: **Final Exam**

Summary of Lecture Material for Chem. 1480 (R.D. Coalson)

Part 1: Molecular Quantum Mechanics and Spectroscopy

1) HistoryBackground. Summary of Classical Mechanics (point mass, trajectory, Newton's Equations, force, potential energy = work, conservation of energy); Failures of Classical Physics: i) Blackbody Radiation (Wien's Law, Stefan Law, UV catastrophe, Planck's formula), ii) Photoelectric Effect, iii) Davisson-Germer Expt.: deBroglie hypothesis, wavelength; Atomic/Molecular Spectra: discrete lines, Bohr transition frequency rule); Emission spectra of the H-atom: Rydberg formula, Bohr atom.

2) QM-Principles. Observables and Linear Operators; Superposition states; Probability density from the wavefunction; Expectation Values; The Heisenberg Uncertainty Principle; assembling Operators from the fundamental x,p operators; the Hamiltonian (total energy operator) and the time-independent Schrodinger Eq.; Techniques and Applications, first example: The 1-d Particle in Box.

3) FEM_2dPB_HO. Techniques and Applications continued: Free Electron Model of pi-bonding in conjugated hydrocarbons; 2D Particle in Box; 1D Harmonic Oscillator (+ application to vibrational motion in a diatomic, infrared spectrum).

4) GlobalWarm_BlackBod. Use of blackbody radiation model and infrared (vibrational) absorption to frame discussion of Global Warming; description of statistics/data processing issues involved: the Signal and the Noise.

5) P-on-Sphere. Particle on Sphere (rigid rotor); energy eigenfunctions and eigenvalues; application to rotational (microwave) spectroscopy of diatomic molecules.

6) H-atom. Hydrogen(ic) atom primer: electronic state wavefunctions, energy levels, probability density, expectations values.

7) AtomsMolecs. Brief survey of electronic structure of multi-electron atoms; Aufbau Principle. Brief introduction to molecular electronic structure: molecular orbitals; the chemical bond, as illustrated through the H2+ molecule ion.

8) Spectroscopy. Brief Survey of the theory of Molecular Spectroscopy: rotational, vibrational, electronic (vibronic, including absorption and emission/fluorescence), covering selection rules and energy level/spectral line patterns.

Part 2: Statistical Mechanics

9) SMstart. Boltzmann probability distribution; illustration with a 1D harmonic oscillator energy ladder.

10) SMinAct. Stat. Mech. in action. Elementary examples: 2-level system (spin in magnetic field), harmonic oscillator, particle in a 1D box (… precursor to center of mass translational motion); partition function; extraction of internal energy; Gibbs (statistical) entropy; Helmholtz free energy in terms of the partition function; Statement/illustration of Classical Equipartition Theorem.

11) ComposSys. Partition function for a composite system: distinguishable subsystems and indistinguishable subsystems (Boltzmann statistics).

12) SakTet+EinHC. Sakur-Tetrode formula for absolute entropy of a monatomic ideal gas; Einstein heat capacity of solids.

13) diatomics. Stat. mech. treatment of ideal gas diatomic molecules. (Focus on rotational and vibrational motion.)

14) ChemEquil. Chemical equilibrium constants from the atomic/molecular partition function. Illustration with ideal gas reactions involving atoms and diatomic molecules.

15) PolyIdGas. Stat. mech. treatment of polyatomic ideal gas. (Focus on rotational and vibrational motion.)

16) PolyEquilConst. Chemical equilibrium constants from molecular partition functions for reactions involving polyatomic gases.

17) NonIdGasTherm. Van der Waals gas: pressure-volume curve; Maxwell equal areas construction.

18) LattGas. Lattice models of surface adsorption and binary liquid mixtures. Random mixing approx. to the partition function; phase transitions (coexistence).