

FINAL EXAM MATERIAL

Remember to bring a Scientific Calculator to the Exam

DATE: Monday, May 9, 2016, 10:30 AM to 1:30 PM

I haven't yet begun preparing the exam, but estimate that it will be approximately 40-45% from "old" material (covered on Exams 1-3) and 55-60% from new material:

Chap. 8: Latter part on Heteronuclear Diat. Molecules (Slides #70-#82)
Chaps. 9 and 10: Parts of each chapter are excluded - See below

Grading: I will not attempt to make the total number of points equal to 100 or 200, but will adjust to a percentage. For example, let's say there are 150 points on the test. The procedure will be (using a score of 140 as illustration):

1. Convert to % by: $\text{Score} \times 100/150 = 140 \times 100/150 = 93.3\%$.
2. If necessary, there might be an additive adjustment to the above score. (no adjustment was needed last year)

The normalized grade (e.g. 93.3% in the example) will be your grade on the final exam. Then, as discussed often, if one of your earlier test grades is less than the Fin. Exam. grade, the earlier grade will be dropped and the Fin. Exam score will be counted twice. If your Fin. Exam. grade is lower than all of your earlier test grades, then it will count only once, and all of your earlier test scores will be used.

Below, I list material from Exams 1-3 and Chaps. 9 and 10, which you can **SKIP**; i.e. the material will not be on the final.

MATERIAL TO SKIP

Exam 1: SKIP

#2: DeBroglie Wavelength

#3: Simplify complex expression

#4: Heisenberg Uncertainty Principle

#6: Wavefunction for a free particle

Exam 2: SKIP

#1: Solving Differential Equation

#2: Anharmonic Vibrations

Exam 3: SKIP

#1(b) Symmetric and Antisymmetric wavefunctions

(c) Normalized Slater Determinant

(d) Diatomic electron configurations

#6: Part (a) Hamiltonian in MKS Units

New Material:

Chaps. 8(Heteronuc. Diatomics) + Chap. 9 + Chap. 10
Material to SKIP

Chapter 8: Skip Stat. Thermo (Slides #83-end)

Chapter 9: SKIP

As noted in class, and in the PP, you are **NOT** responsible for any of the SCF-LCAO Equations (Slides #27 - #35)

You are **NOT** responsible for interpreting the output of a QM run (Slides #37-#53)

You are **NOT** responsible for the latter applications of QM, starting with Slide #120 through the end of the chapter.

Note: You should know the thermodynamic formulas on Slide #102. They may well be needed, but will not be given.

Chapter 10: SKIP

Part A - Slide #39 + HW #2: Number of electrons contributed by heteroatom).

Part A - Slides #46 - #54: Semiempirical methods for sigma bonded systems.

Part B - Slides #22 through end - Use of symmetry in Simplifying MO Calculations. Because we are not presenting this topic this year, you can skip HW #8 as well as Problem #10 on last year's Final Exam.

Note that you ARE responsible for the earlier slides, showing the application of symmetry to determine UV/Visible Absorption Selection Rules.