CHM 3411 Problem Solving Session 4-16-2018

<u>On Exam 3 Topics</u>

- Chapter 10, Sections D-E
- Including computational chemistry (last topic in 10E + extra handout posted to be website → at end is list of exactly what you need to know)

Main points

- Be able to draw a schematic MO energy level diagram for a heteronuclear diatomic, knowing I (ionization energy) for each atom.
- Know what the experimental data that the Pauling and Mulliken electronegativies are based on. Be able to calculate either one.
- Know the meaning of the variation principle
- Be able to apply the Hückel method.
- Be able to determine E_{π}, E_{bf}, and E_{dl} from the MO energy level diagram.
- I put a document on computational chemistry on my website some time ago. The end lists precisely those things for which you are responsible.

Heteronuclear diatomic MO question

Given: Iodine I_1 =10.5 eV; Fluorine: I_1 =17.4 eV

- (1) Sketch the MO energy level diagram, (2) Determine electron configuration, (3) Determine whether IF will have shorter bond than IF^- or IF^+.

Electronegativity question

- Why is there more than one definition of electronegativity?
- What experimental data are Pauling electronegativities based on?
- What experimental data are Mulliken electronegativies based on?

Variation principle question

- In words, what is the meaning of the variation principle?
- What equation expresses the variation principle?
- What is the importance of the variation principle?

Hückel MO question (from PS 10)

- Apply Hückel MO theory to the allyl radical(CH_2CHCH_2), and use it to explain the unusual stability of the allyl radical.