Name
Section
Rec TA

Ch 1a, Problem Set Five
Due Friday, Oct. 27, 2006
at 4 PM in the Drop Box

Problems 2 and 4 are designated (☎) as 'no collaboration' problems.

1. (15 Points) You have just completed an experiment where you measured the first ionization energies of consecutive elements. Unfortunately, as you are perusing your results over lunch, you smear lutefisk, a Norwegian delicacy of fish soaked in lye underground for two weeks, on your notebook, rendering half of the page illegible. Rather than redo the experiment, which took you the better part of a day, you decide to apply your Ch1a knowledge to reconstruct the data. You remember that the first entry has the lowest atomic number of the list. As the list goes up alphabetically, the atomic numbers increase consecutively, so that the last entry has the highest atomic number. What is element L on this list? Explain your reasoning.

Element	Ionization Energy
A	499
B	735
C	580
D	788
E	1010
F	1002
G	1248
H	1523
I	420
J	593
K	635
L	664

☎ 2. (15 Points) Out of each pair, which ion has the smaller radius? No credit will be given unless you explain each inequality in terms of screening or electronic configurations.

a. (5 Pts) Cs^{+} , Sr^{2+}
b. (5 Pts) (5 Pts) Sr^{2+} , Nb^{2+}
c. (5 Pts) Br^{-} , Kr

3. (15 Points) Out of each pair, which neutral element has the lower ionization energy? Explain each answer with screening and/or electronic configurations for full credit.

a. (5 Pts) Na , Mg
b. (5 Pts) Zn , Ge
c. (5 Pts) Mg , Ne

☎ 4. (10 Points) Making covalent bonds to the silicon surface has important implications for the silicon device industry. Calculate the difference in Pauling electronegativity (page 56, Gray) for each Si-R bond given and rank each bond from the most ionic (greatest difference in electronegativity) to most covalent (least difference).

Si-Cl, Si-OH, Si-H, Si-CH_3, Si-SiH_3, Si-F

5. (20 Points) In lecture, electron shielding was qualitatively addressed. In 1930, J.C. Slater developed a semi-quantitative model for shielding which works well for the main group elements and the first row of the transition metals. His model calculates an effective nuclear charge, Z^*, seen by an electron as a result of the shielding from the remaining electrons. Z^* is calculated from the nuclear charge, Z, and a shielding parameter, S.

$$Z^* = Z - S \tag{1}$$

The shielding parameter, S, is calculated using the following rules:

- *All* electrons are divided into groups as follows:

Group One:	{1s}	Group Six:	{4d}
Group Two:	{2s, 2p}	Group Seven:	{4f}
Group Three:	{3s, 3p}	Group Eight:	{5s, 5p}
Group Four:	{3d}	*Electrons in higher groups (5d, 6s, etc)*	
Group Five:	{4s, 4p}	*are not considered in this model…*	

- Choose an electron for which you wish to calculate, S, and Z^*. This is often the "last" valence electron, or the first electron that would be ionized out of the atom.

- If the chosen electron is an *s* or *p* electron:
  a. Electrons in the same group as the chosen electron each contribute 0.35 to S.
  b. Electrons 1 group lower than the chosen electron (s, p, or d) contribute 0.85 to S.
  c. Electrons 2 groups *or lower* than the chosen electron contribute 1.00 to S.
  d. All other electrons may be ignored.

- If the chosen electron is a *d* or *f* valence electron:
  a. Electrons in the same group as the "last electron" contribute 0.35 to S.
  b. Electrons in groups lower than the "last electron" contribute 1.00 to S.
  c. All other electrons may be ignored.

Consider this sample calculation of Z^*, for the outermost electron of oxygen:

- Electron Configuration: $1s^2 2s^2 2p^4$. The "last electron" is in a 2p orbital (group two), therefore there are $1s^2 2s^2 2p^3$ remaining electrons which shield this electron.
- The 3 2p and 2 2s electrons are all in group two which is the same group as this last electron. They all contribute 0.35 to S. The 1s electrons are 1 group lower (group one) and both of these contribute 0.85 to S. So $S = 2x.85 + 5\ x.35 = 3.45$
- $Z^* = Z - S = 8 - 3.45 = 4.55$. So a 2p electron in Oxygen only "sees" 4.55/8 or about 57% of the total nuclear charge.

a. (5 Pts) Calculate Z^*, and Z^*/Z for a *3p* electron of Silicon.
b. (5 Pts) Calculate Z^*, and Z^*/Z for a *2p* electron of Carbon.
c. (5 Pts) From your answers in a. and b., Comment on the correlation between S, Z^*, and the periodic trends in ionization energy.
d. (5 Pts) On the basis of Z^*, determine which orbital an electron removed from in the ionization of Ag to Ag^+. Give the electron configuration of Ag^+. *Hint*: calculate Z^* for a number of different "last electrons". Why is one removed over another? Explain.

6. (25 Points, 5 Each) For each of the following molecules, draw a Lewis dot structure. Show any significant resonance structures and formal charges.

   a. $[OCHCH_2]^-$
   b. NO_2
   c. O_3 *(hint: not a triangle)*
   d. SOF_6 *(hint: one F attached to O)*
   e. SO_3