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Chemistry 4A Midterm 2

Please write your answers with pen or dark pencil. Answers will only be graded within the boxes below each question. To receive full credit, please write the equation that you use to answer the question, and then give your answers in numerical values.

1. (20 pts) The following concerns the description of electron orbitals in the H-atom.

   (a) For n=2 energy level of the H-atom, what are all the allowed quantum numbers of the electron? When possible, state what the quantum number represents classically. Also state which do not have a classical analogy.

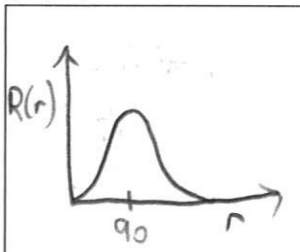
$l = 0, 1$ Magnitude of angular momentum

$m_l = -1, 0, 1$ Extent of Angular momentum in the z direction

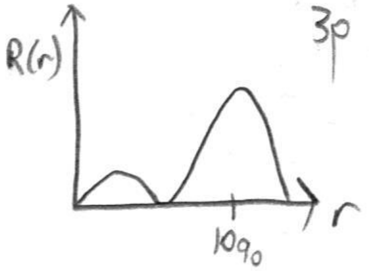
$s = +\frac{1}{2}, -\frac{1}{2}$ No classic analogy

$n = 2$ Energy level

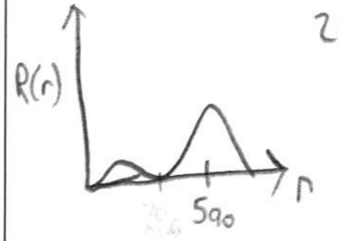
   (b) Graph the radial distribution functions for 1s, 2s, 2p, and 3p orbitals. On each graph, locate on the radial axis the most probable location of the electron.



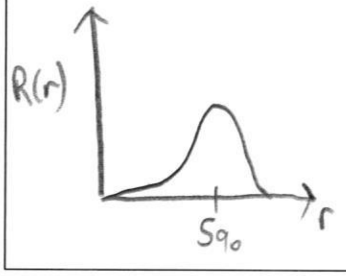
1s



2s



$a_0 = 53$ Angstroms



(c) If the electron is in the 3p orbital, how many angular nodes (either an axis or a plane) does it have? How many radial ones?

It has one angular node and one radial node

$$\text{Radial}\begin{cases} n = n_r + \ell + 1 \\ 3 = n_r + 1 + 1 \\ n_r = 1 \end{cases}$$

$$\text{Angular}\begin{cases} n_{Total} = n - 1 \\ n_A + n_r = 3 - 1 \\ n_A + 1 = 2 \quad n_A = 1 \end{cases}$$

2. (10 pts) Using a good approximation for the Z_{EFF} of each element, calculate the first ionization energies of H, Li, Na, and K. You can take R_H to equal 1200 kJ/mol.

$$I = -E_n = \frac{Z_{eff}^2 \cdot R_H}{n^2}$$

H: $Z_{EFF} = 1$

$n = 1$

$\boxed{I = 1200\ \text{kJ} \cdot \text{mol}}$

Li: $Z_{EFF} = 1$

$n = 2$

$I = \frac{1200\ \text{kJ/mol}}{4} = \boxed{300\ \text{kJ/mol}}$

Na: $Z_{EFF} = 1$

$n = 3$

$I = \frac{1200\ \text{kJ/mol}}{9} = 133.33\ \text{kJ/mol}$ 1200 has 2 sigfigs

$= \boxed{130\ \text{kJ/mol}}$

K: $Z_{EFF} = 1$

$n = 4$

$I = \frac{1200\ \text{kJ/mol}}{16} = \boxed{75\ \text{kJ/mol}}$

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3. (6 pts) Explain, in terms of ionization energies and electron affinities, why the electronegativity of F is so much larger than its next door neighbor, Ne.

Electronegativity = Ionization energy - Electron Affinity

~~[illegible]~~ Neon has all of its 2s and 2p electrons screening the next electron that it takes*, so Neon's electron affinity will be low. Fluorine has a ~~[illegible]~~ low EA since its 2s and 2p electrons won't screen much of the next electron it takes that joins the 2p orbital.

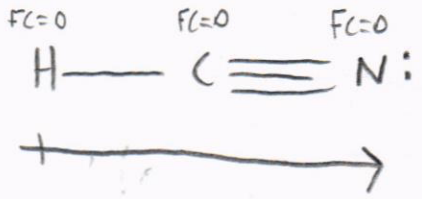
Thus, since lower electron affinity means higher electronegativity and the differences between their EA is much more significant than that of the ionization energy^{*_2} ($\Delta Z_{eff} = 1$) and $I \propto Z_{eff}^2$, Fluorine has a higher electronegativity.

*which will be in the 3s orbital.

$*_2$ Neon's I_E is greater that Fluorine's

4. (10 pts) Consider the HCN molecule for the following questions.

(a) Draw the Lewis dot structure, including all bonds, lone pairs, and formal charges.

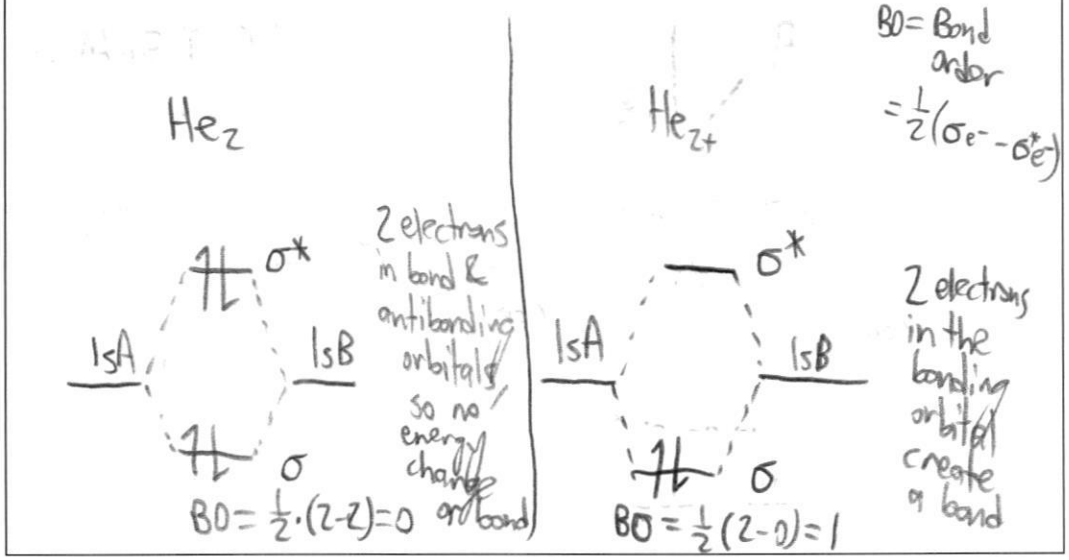


(b) Do you expect this molecule to be polar? If so, draw an arrow on the lewis structure indicating the direction of the net polarity (arrowhead towards negative charge).

I expect it to be polar.

5. (18 pts) The He_2 molecule is not stable, whereas the He_2^{2+} molecular ion is stable.

(a) Draw a molecular orbital energy level diagram to explain this and calculate He_2^{2+}'s bond order.



2 electrons in bond & antibonding orbitals so no energy change or bond

$BO = \frac{1}{2}\cdot(2-2) = 0$

BO = Bond order $= \frac{1}{2}(\sigma_{e^-} - \sigma^*_{e^-})$

2 electrons in the bonding orbital create a bond

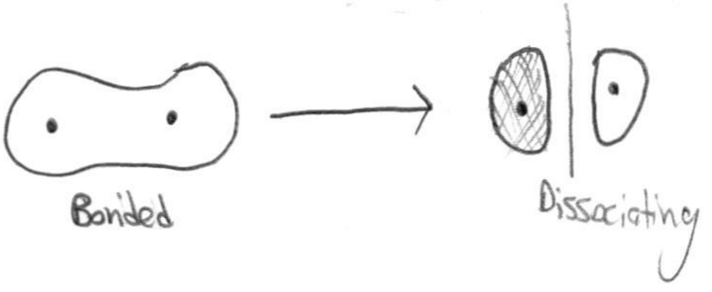
$BO = \frac{1}{2}(2-0) = 1$

(b) If it takes 100 kJ/mol to dissociate He_2^{2+} by exciting an electron to the antibonding orbital, how much lower is the bonding orbital from the final, dissociated state of the two He ions ?

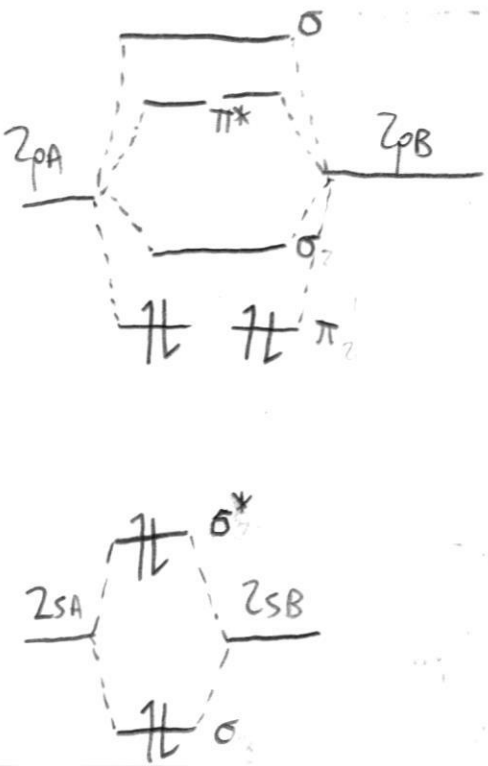
$$D_E = \frac{100\,\frac{kJ}{mol}}{2} = \boxed{50\,\frac{kJ}{mol}}$$

lower

(c) Draw the wavefunction of the excited electron right before it dissociates. Show any sign differences by shading and any nodal planes by a line.



6. (20 pts) Draw the molecular orbital energy level diagram for C_2 (where there is s-p mixing) and fill in the valence electrons. In the diagram, label atomic energy levels with their atomic orbitals and the molecular energy levels with σ, π, σ^*, and π^*. Then answer the following questions:



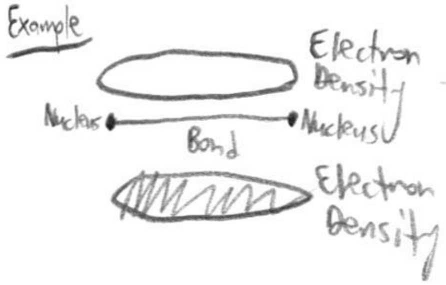
(a) Calculate its bond order.

Bond Order = $\frac{1}{2}(6-2) = 2$

$BO = \frac{1}{2}(\sigma e^{-} - \sigma^{*} e^{-})$

(b) What type of bond leads to the stability of the C_2 diatomic molecule? Where is the electron probability density located with respect to the bond?

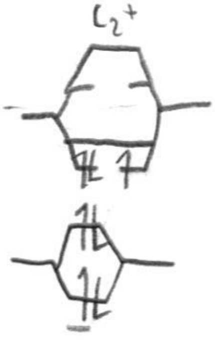
The bond is a π bond, and it is a double bond. The electron probability is located parallel to the bond.



(c) Is the molecule paramagnetic or diamagnetic?

The molecule is diamagnetic. (All electrons are paired in molecular orbitals)

(d) Compare its bond strength to C_2^+ and C_2^-.



$BO = \frac{1}{2}(5-2) = \frac{3}{2}$

$BO = \frac{1}{2}(7-2) = \frac{5}{2}$

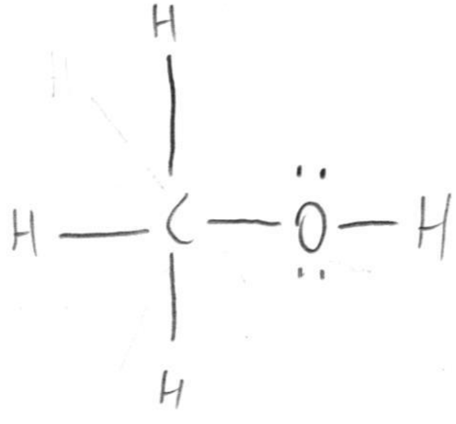
C_2^+ is weaker than C_2

C_2^- is stronger than C_2

(Higher Bond order is stronger)

7. (16 pts) The following concern the molecule methanol, CH_3OH:

(a) Draw out the Lewis structure, including lone pairs and bonds.



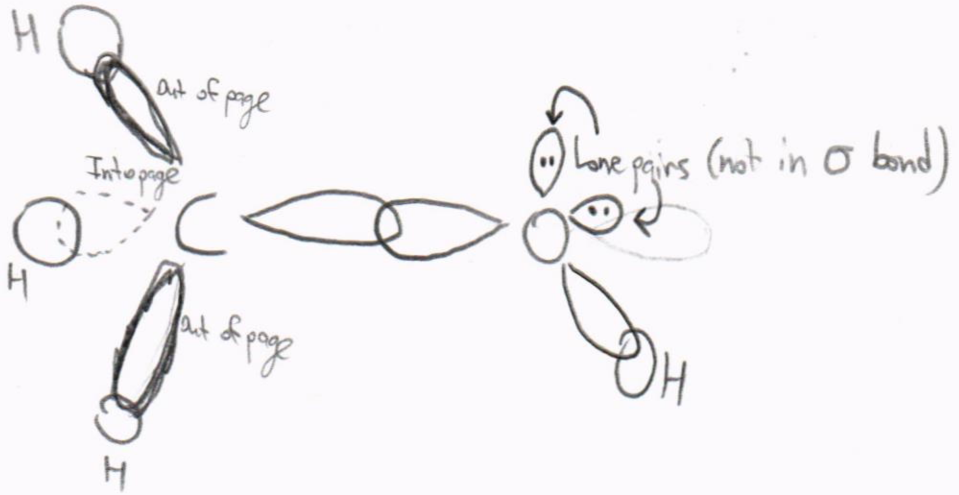
FC=0 for all atoms

(b) What is the VSEPR predicted geometry for C and O?

C: e^- geometry is tetrahedral (predicted)
molecular geometry is tetrahedral (actual)

O: e^- geometry is tetrahedral (predicted)
molecular geometry is bent (actual)

(c) For this geometry, draw out the σ bond framework for C and O and state how the s-p orbitals are hybridized.



C has sp3 hybridization (one 2s electron is excited to the 2p orbital, 1 2s and 3 2p orbitals combine into 4 sp_3 orbitals)

O has sp_1 hybridization (1 2p and 1 2s orbital combine into 2 sp_1 orbitals)

(2 2p orbitals are left behind and hold the lone pairs.