Name:_____ Student Number:_____

CHEM 1001 A, N and T Midterm Test #2
November 6, 2015
Calculators Allowed
Make sure this test has 7 pages. You may tear off the last page.

Part A. Answer each of the six questions with a few sentences or equations where necessary. (5 Marks each)

1. In the photoelectric effect, the kinetic energy of the ejected electron is equal to the photon energy minus what quantity?

   The kinetic energy of the ejected electron is equal to the photon energy minus **the binding energy of the electron**.

2. The ground state electronic configuration for silver (Ag) is predicted by AUFBAU to be $[Kr]\ 5s^2\ 4d^9$. The actual configuration is different. What is it and why is it different from the predicted configuration?

   It is actually $[Kr]\ 5s^1\ 4d^{10}$ because this configuration contains a half-filled 5s subshell and a filled 4d subshell, which is a lower energy configuration that a filled 4s and a 9/10ths filled 3d subshell.

3. Why is the second ionization potential of an atom always greater than the first?

   The first ionization potential is the energy required to remove an electron from a singly charged cation (as in $X \rightarrow X^+ + e^-$). The second is the energy required to remove an electron from a doubly charged cation (as in $X^+ \rightarrow X^{2+} + e^-$). There is more attractive potential energy between an electron and a doubly charged cation.

4. Why does a double or triple bond contain at most one sigma (σ) bond?

   Once a sigma bond is formed, any p-orbitals remaining after hybridization must be parallel to one another. The only way they can overlap is sideways, resulting in pi-bonds.

5. Why is BH_3 not polar? Why is NH_3 polar?

   BH_3 is trigonal planar with 120^o bond angles. Although each B-H bond is polar, these dipoles cancel each other out. NH_3 is a trigonal pyramidal molecule, and the dipole do not cancel each other out, resulting in a net dipole.

6. How does the bandgap between the HOMO and LUMO in a molecule affect the colour of the compound?

   If the bandgap is large, the molecule will only absorb photons in the UV portion of the spectrum, which we cannot see, so the compound will appear to be colourless. If the bandgap is smaller, absorption of photons in the VIS portion of the spectrum is possible, resulting in colour.

Part B. Answer any three of the following four questions (B1, B2, B3, B4). If you answer all four, the best three answers will count. (20 marks each)

B1. (a) Calculate the energy (in kJ mol^{-1}) of photons resulting from the lowest energy transition of an electron in the Lyman series of the hydrogen atom. Transitions in the Lyman series terminate at m = 1.

$$\frac{1}{\lambda} = R\left[\frac{1}{m^2} - \frac{1}{n^2}\right]$$

The lowest energy transition must originate at n = 2, thus:

$$\frac{1}{\lambda} = 0.01097\ nm^{-1}\left[\frac{1}{1^2} - \frac{1}{2^2}\right]$$

$$= 0.00823\ nm^{-1}$$

$$\lambda = \frac{1}{0.00823\ nm^{-1}} = 121.5\ nm$$

$$E = \frac{hc}{\lambda} = \frac{6.63\times10^{-34}\ J\,s\,(3.00\times10^{8}\ m\ s^{-1})}{121.5\times10^{-9}\ m} = 1.64\times10^{-18}\ J\ (per\ photon)$$

$$\times 6.02\times10^{23}\ mol^{-1} = 985142\ J\ mol^{-1} = 985.1\ kJ\ mol^{-1}$$

(b) $NO_{2(g)}$ is an important species in the formation of smog in large cities. The N-O bond dissociation energy is 279 kJ mol^{-1}. Calculate the longest wavelength (in nm) of light that can break this bond.

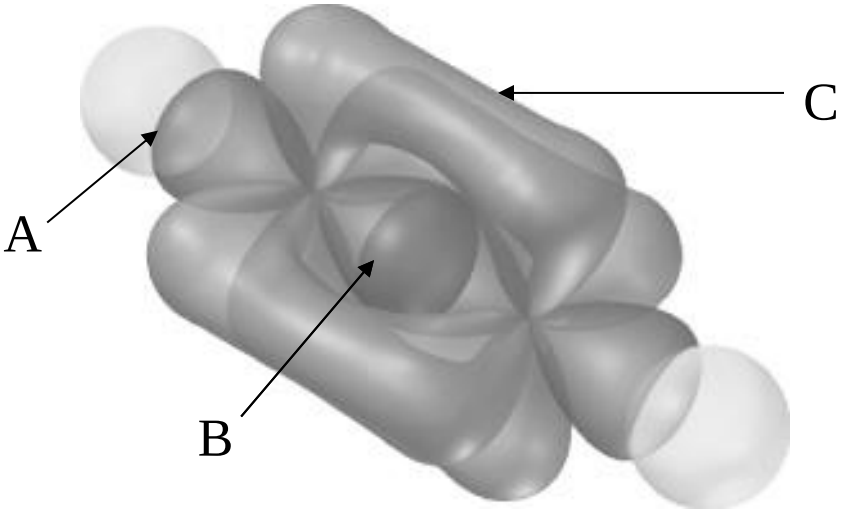
$$E = 279000\ J\,mol^{-1} = \frac{279000 J\,mol^{-1}}{6.02\times10^{23}\ mol^{-1}} = 4.63\times10^{-19} J\ (per\ photon)$$

$$\lambda = \frac{hc}{E}$$

$$= \frac{6.63\times10^{-34} J\ s\ (3.00\times10^{8}\ ms^{-1})}{4.63\times10^{-19} J} = 4.29\times10^{-7}\ m$$

$$= 429\ nm$$

B2. (a) Use the diagram of an acetylene molecule, C_2H_2, to fill in the blanks.



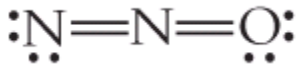
(i) '**A**' is a σ bond, formed by the overlap of a s atomic orbital of the H atom with a sp hybrid orbital of the C atom.

(ii) '**B**' is a σ bond, formed by the overlap of a sp hybrid orbital of one carbon with a sp hybrid orbital of the other carbon.

(iii) '**C**' is a π bond, formed by the overlap of a p orbital of one carbon with a p orbital of the other carbon.

(iv) C_2H_2 has a (circle one) SINGLE DOUBLE (TRIPLE) carbon-carbon bond

(b) Calculate and enter the formal charge of each atom in the box below each atom of each structure of N_2O.

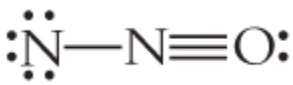


-1	**+1**	**0**

(Structure A)

0	**+1**	**-1**

(Structure B)



-2	**+1**	**+1**

(Structure C)

Based on formal charges, the **least** likely structure is (circle one)

A B (C)

B3. (a) Use VSEPR theory to predict the shape of BrF_3. Wrong name = zero marks.

7 + (3 x 7) = 28 electrons. Arranging the three F atoms around the Br atom and making two-electron bonds uses six electrons. Completing the octets on the F atoms uses another 18 for a total of 24. The last four electrons are placed as two lone pairs on the central Br atom. The shorthand notation is therefore AX_3E_2, which is **T-shaped**.

(b) Use VSEPR theory to predict the shape of $AsCl_3^+$. Wrong name = zero marks.

5 + (3 x 7) - 1 = 25 electrons. Arranging the three Cl atoms around the As atom and making two-electron bonds uses six electrons. Completing the octets on the Cl atoms uses another 18 for a total of 24. The last electron is placed (alone) on the central Br atom. The shorthand notation is therefore AX_3E, which is **trigonal pyramidal**.

(c) Use the molecular orbital diagram for C_2 below to answer the following questions:

(i) Calculate the bond order of C_2.

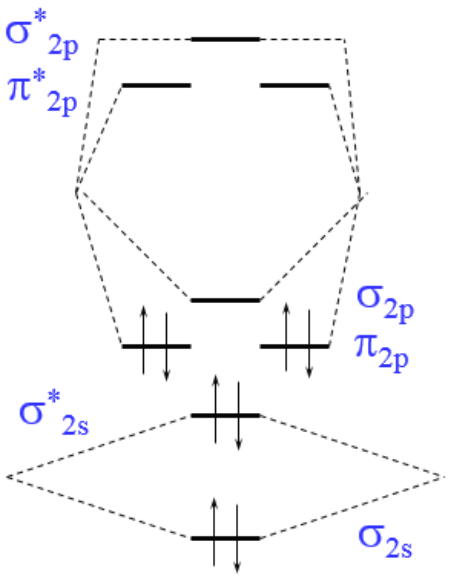
Bond order = (6 – 2)/2 = 2

(ii) Is C_2 paramagnetic or diamagnetic? Why?

C_2 is diamagnetic because all electrons are paired.

(iii) Is C_2^+ paramagnetic or diamagnetic? Why?

C_2^+ is paramagnetic because it has one unpaired electron (in the π_{2p} MO).



(iv) Is the bond length of C_2^+ greater or less than that of C_2? Why?

Making C_2^+ requires removing an electron from the highest energy occupied MO, which is a π (bonding) MO. The bond order therefore decreases, resulting in a longer bond in C_2^+ than in C_2.

(v) Is the bond energy of C_2^- greater or less than that of C_2? Why?

Making C_2^- requires adding an electron to the lowest energy unoccupied MO, which is the σ_{2p} (bonding) MO. The bond order therefore increases, resulting in a larger bond energy in C_2^- than in C_2.

B4. **C**alculate the lattice energy (in kJ/mol) of $BaH_{2(s)}$ given the following data:

ΔH^o_f ($BaH_{2(s)}$)	-40.9 kJ mol^{-1}
BDE (H_2)	436 kJ mol^{-1}
EA (H)	-73 kJ mol^{-1}
H_{sub} ($Ba_{(s)}$)	+175.4 kJ mol^{-1}
I_1 (Ba)	+502 kJ mol^{-1}
I_2 (Ba)	+963 kJ mol^{-1}

$Ba_{(s)} \rightarrow Ba_{(g)}$	+175.4 kJ mol^{-1}
$Ba_{(g)} \rightarrow Ba^{+}_{(g)} + e^-$	+502 kJ mol^{-1}
$Ba^{+}_{(g)} \rightarrow Ba^{+2}_{(g)} + e^-$	+963 kJ mol^{-1}
$H_{2(g)} \rightarrow 2\ H_{(g)}$	+436 kJ mol^{-1}
$2\ H_{(g)} + 2\ e^- \rightarrow 2\ H^-_{(g)}$	2(-73) = -146 kJ mol^{-1}
$Ba^{+2}_{(g)} + 2\ H^-_{(g)} \rightarrow BaH_{2(s)}$	–U (+U = lattice energy)

Adding all of the above reactions gives:

$Ba_{(s)} + H_{2(g)} \rightarrow BaH_{2(s)}$
which has an energy of –40.9 kJ mol^{-1}, since this is the formation of $BaH_{2(s)}$ from the elements

Therefore, –U = –40.9 – (175.4+502+963+436–146) = –1971.3
U = +1971.3 kJ mol^{-1}

Part A	B1	B2	B3	B4	Total / 90