

Name: _____

Student Number: _____

CHEM 1001 A, N and T Midterm Test #2

November 17, 2017

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. (5 Marks each)

1. What is the strongest type of intermolecular force between HCl and CCl₄?

HCl is a dipole. CCl₄ is not polar. The strongest force is therefore dipole-induced dipole.

2. What kind of hybrid orbitals are used by the central S atom to bond with the terminal F atoms in SF₂? How do you know?

$6 + 2(7) = 20$ valence electrons. Connecting the F atoms to the S atom with single bonds and completing the octets on the F atoms uses 16 electrons. Thus, there are also two lone pairs on the S atom. The S atom thus has four electron groups around it (i.e. has a steric number of four), and must therefore be using sp³ hybrid orbitals.

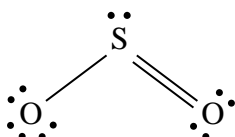
3. Why does Fe have two common ions, Fe²⁺ and Fe³⁺?

The electronic configuration for Fe is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$. The two 4s electrons are at the highest energy and so are most easily removed, resulting in Fe²⁺. Further removing one of the 3d electrons results in a half-filled 3d subshell, which is very stable, resulting in Fe³⁺.

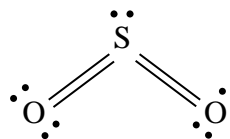
4. Why is BH₃ not polar? Why is NH₃ polar?

BH₃ is trigonal planar with 120° bond angles. Although each B-H bond is polar, these dipoles cancel each other out. NH₃ is a trigonal pyramidal molecule, and the polar bonds do not cancel each other out, resulting in a net dipole.

5. Which of the two structures of SO₂ (A or B) is more likely, based on formal charges? Why?



A



B

In structure A, the formal charges on the left hand oxygen and on the S atom are -1 and +1 respectively. In structure B, all formal charges are zero. Thus, structure B is more likely.

6. An electron is removed from a molecule and the bond length decreases. What can be concluded about the molecular orbital of the electron that was removed? Why?

The electron must have been in an anti-bonding molecular orbital. Removing it increases the bond order, which decreases the bond length.

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. [20 marks] (a) Use the following data to calculate the third ionization potential of Sc (in kJ mol^{-1}). You must write out each reaction correctly [10 marks], and do the math correctly [10 marks] to receive full marks.

$$\Delta H_{\text{f}}^{\circ}(\text{ScCl}_{3(\text{s})}) = -922.9 \text{ kJ mol}^{-1}$$

$$\Delta H_{\text{sub}}^{\circ}(\text{Sc}_{(\text{s})}) = 388.7 \text{ kJ mol}^{-1}$$

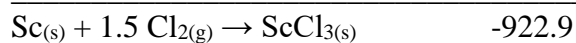
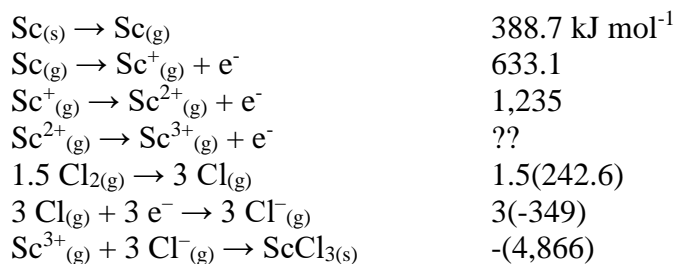
$$I_1(\text{Sc}_{(\text{g})}) = 633.1 \text{ kJ mol}^{-1}$$

$$I_2(\text{Sc}_{(\text{g})}) = 1,235.0 \text{ kJ mol}^{-1}$$

$$\text{Lattice energy of } \text{ScCl}_{3(\text{s})} = 4,866 \text{ kJ mol}^{-1}$$

$$\text{Bond dissociation energy of } \text{Cl}_{2(\text{g})} = 242.6 \text{ kJ mol}^{-1}$$

$$\text{Electron affinity of Cl} = -349 \text{ kJ mol}^{-1}$$



Thus, the third ionization potential of Sc can be calculated by difference:

$$\begin{aligned} I_3(\text{Sc}_{(\text{g})}) &= -922.9 - (388.7 + 633.1 + 1,235 + 1.5(242.6) + 3(-349) - 4,866) \\ &= 2,369 \text{ kJ mol}^{-1} \end{aligned}$$

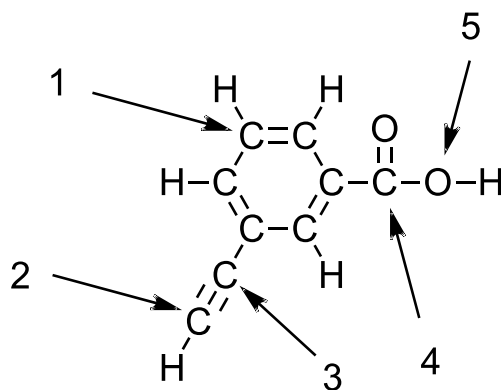
B2. (a) [5 marks] Predict the shape of XeF_2 . Wrong name of shape = zero marks!

$8 + 2(7) = 22$ valence electrons. Connecting the F atoms to the Xe atom with single bonds and completing the octets on the F atoms uses 16 electrons. Thus, there are also three lone pairs on the Xe atom. The shorthand notation for this molecule is therefore AX_2E_3 , which is a **linear** molecule.

(b) [5 marks] Predict the shape of ClF_4 . Wrong name of shape = zero marks!

$7 + 4(7) = 35$ valence electrons. Connecting the F atoms to the Cl atom with single bonds and completing the octets on the F atoms uses 32 electrons. Thus, there is also a lone pair and a single electron on the Cl atom. The shorthand notation for this molecule is therefore AX_4E_2 , which is a **square planar** molecule.

(b) [10 marks] What hybridization is each of the five indicated atoms using in the molecule shown below?



Atom 1: sp^2 ___ Atom 2: sp ___ Atom 3: sp^3 ___ Atom 4: sp^2 ___ Atom 5: sp^3 ___

(Note that there are two implicit lone pairs on atom 5!)

B3. (a) Use the molecular orbital diagram for the B_2 molecule below to answer the following questions:

(i) [1 mark] Calculate the bond order of B_2 .

$$\text{Bond order} = (4 - 2)/2 = 1.0$$

(ii) [1 mark] Is B_2 paramagnetic or diamagnetic? Why?

B_2 is paramagnetic because of the unpaired electrons in the π_{2p} molecular orbital.

(iii) [2 marks] Calculate the bond order of B_2^+

$$\text{Bond order} = (3 - 2)/2 = 0.5$$

(iv) [2 marks] Which of B_2^- and B_2^{2-} are paramagnetic? Why?

B_2^- is paramagnetic because it would have one unpaired electron.

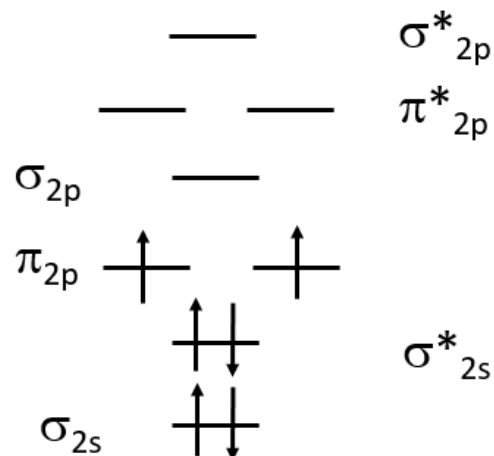
B_2^{2-} would not be because all electrons would be paired up.

(v) [2 marks] Which of B_2 or B_2^+ has the greater bond length? Why?

B_2^+ has the greater bond length because it has the smaller bond order.

(vi) [2 marks] Which of B_2 or B_2^- has the greater bond energy? Why?

B_2^- has a greater bond energy than B_2 because it has a larger bond order.



- (b) [10 marks] Iron metal crystallizes in a body-centred cubic structure and has a density of 7.87 g cm^{-3} . Calculate the radius of an iron atom (in pm). You may use geometry to solve this problem, or the fact that the atoms in a BCC structure occupy 68% of the volume of the unit cell.

Method A: In a BCC unit cell, there are the equivalent of two whole atoms ($1/8$ atom at each corner plus a whole atom in the centre). The mass of the unit cell is therefore:

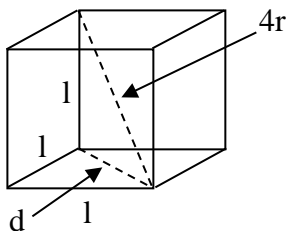
$$m_{\text{unit cell}} = 2 \text{ atoms} \left(\frac{55.85 \text{ g}}{6.02 \times 10^{23} \text{ atoms}} \right) = 1.86 \times 10^{-22} \text{ g}$$

And the volume of the unit cell is therefore:

$$V_{\text{unit cell}} = \frac{\text{mass}_{\text{unit cell}}}{\rho} = \frac{1.86 \times 10^{-22} \text{ g}}{7.87 \text{ g cm}^{-3}} = 2.36 \times 10^{-23} \text{ cm}^3$$

And so the edge length of the unit cell is:

$$l = \sqrt[3]{V_{\text{unit cell}}} = \sqrt[3]{2.36 \times 10^{-23} \text{ cm}^3} = 2.86 \times 10^{-8} \text{ cm}$$



In the diagram above, note that the diagonal through the centre of a BCC unit cell passes through three atoms, and has a length of $4r$:

$$d^2 = l^2 + l^2$$

$$\text{but, } (4r)^2 = l^2 + d^2 = 3l^2$$

$$\text{Thus, } 16r^2 = 3l^2, \text{ or } r = \frac{l\sqrt{3}}{4} = \frac{2.86 \times 10^{-8} \text{ cm}(\sqrt{3})}{4} = 1.24 \times 10^{-8} \text{ cm} = 124 \text{ pm}$$

Method B: Density of the metal is 7.87 g cm^{-3} .

The volume occupied by one gram of iron is therefore $V = \frac{1}{7.87 \text{ g cm}^{-3}} = 0.1271 \text{ cm}^3 \text{ g}^{-1}$

and per mole, it is $0.1271 \text{ cm}^3 \text{ g}^{-1} \times 55.85 \text{ g mol}^{-1} = 7.098 \text{ cm}^3 \text{ mol}^{-1}$

but the atoms occupy only 68% of this space, thus the volume occupied by one mole of the atoms themselves is $0.68(7.098 \text{ cm}^3 \text{ mol}^{-1}) = 4.827 \text{ cm}^3 \text{ mol}^{-1}$

and per atom, it is $\frac{4.827 \text{ cm}^3 \text{ mol}^{-1}}{6.02 \times 10^{23} \text{ mol}^{-1}} = 8.02 \times 10^{-24} \text{ cm}^3$

Each atom is a sphere of radius r , and volume = $(4/3)\pi r^3$

$$\text{Thus, } r = \sqrt[3]{\frac{3V}{4\pi}} = \sqrt[3]{\frac{3(8.02 \times 10^{-24}) \text{ cm}^3}{4\pi}} = 1.24 \times 10^{-8} \text{ cm} = 124 \text{ pm}$$

- B4.** (a) [10 marks] Tantalum (Ta) crystallizes in some type of cubic unit cell. The edge length of the unit cell is 331 pm. The density of tantalum metal is 16.7 g cm^{-3} . What type of cubic unit cell does tantalum form?

$$\text{Volume of the unit cell} = V = (331 \times 10^{-10} \text{ cm})^3 = 3.63 \times 10^{-23} \text{ cm}^3$$

$$\text{Mass of unit cell} = m = \rho V = 16.7 \text{ g cm}^{-3} \times 3.63 \times 10^{-23} \text{ cm}^3 = 6.06 \times 10^{-22} \text{ g}$$

$$\text{Mass of one Ta atom} = \frac{180.95 \text{ g mol}^{-1}}{6.02 \times 10^{23} \text{ mol}^{-1}} = 3.01 \times 10^{-22} \text{ g}$$

$$\text{Number of atoms per unit cell} = \frac{6.06 \times 10^{-22} \text{ g / unit cell}}{3.01 \times 10^{-22} \text{ g / atom}} = 2 \text{ atoms / unit cell}$$

Only **BCC (body centered cubic)** has two atoms per unit cell.

- (b) [10 marks] The valence electrons in a Protactinium (Pa) atom are $7s^2 5f^2 6d^1$.

What are the four quantum numbers for each of these five electrons?

One of the 7s electrons: $n = \underline{7}$ $l = \underline{0}$ $m_l = \underline{0}$ $m_s = \underline{+1/2}$

The other 7s electron: $n = \underline{7}$ $l = \underline{0}$ $m_l = \underline{0}$ $m_s = \underline{-1/2}$

One of the 5f electrons: $n = \underline{5}$ $l = \underline{3}$ $m_l = \underline{-3, -2, -1, 0, 1, 2 \text{ or } 3}$ $m_s = \underline{+1/2}$

The other 5f electron: $n = \underline{5}$ $l = \underline{3}$ $m_l = \underline{-3, -2, -1, 0, 1, 2 \text{ or } 3}$ (but different from above) $m_s = \underline{+1/2}$

The 6d electron: $n = \underline{6}$ $l = \underline{2}$ $m_l = \underline{-2, -1, 0, 1 \text{ or } 2}$ $m_s = \underline{+1/2}$