CH301H – Principles of Chemistry I: Honors
Fall 2013, Unique 52195

Exam 1
19 September 2013

Name: Key

You may use any material you wish provided it does not have a heartbeat nor does it connect to a wireless or cellular network.

Honor Code:

"The core values of the University of Texas at Austin are learning, discovery, freedom, leadership, individual opportunity, and responsibility. Each member of the University is expected to uphold these values through integrity, honesty, trust, fairness, and respect toward peers and community."

I certify that the work on this exam is entirely my own.

Signature Date

1. (12 points) Determine whether the following statements are true or false.

a. True False In an ionic bond, electrons are shared between the two atoms.

b. True False Any atom's first ionization energy is < 0 always.

c. True False Electronegativity is defined as the sum of ionization energy and electron affinity.

d. True False Carbon has 8 electrons in its valence shell.

e. True False Sodium is larger than potassium.

f. True False IF_4 (i.e. iodine tetrafluoride) is tetrahedral.

2. (14 points) The following data are available:

Molecule	EN difference	% ionic character
LiF	3.0	88
KF	3.16	80
CsF	3.19	71

In clear, comprehensible English, explain why the % ionic character of this series of molecules goes down while the difference in electronegativity (EN) goes up.

Electronegativity is a qualitative guideline that tells us how much one atom will try to hold onto electrons in a molecule. Dipole moment is an experimentally observed distribution of charge across a region of space (such as the length of a bond). It is from this measurement that % ionic character can be determined. Large differences in EN will be associated with highly ionic molecules, but when comparing molecules of roughly similar ΔEN (such as in this problem), actual differences in % ionic character will be a convolution both of ΔEN and differences in atomic size.

*The first part of this question is almost identical to one of your practice exams. It pays to use all your resources!

3. (30 points) Hydrogen cyanide, HCN, is a strong acid that is a vapor at room temperature.

a) Draw the Lewis dot structure for HCN. Clearly indicate the number of bonds between each atom and the position of any lone electron pairs.

$$H-C\equiv N:$$

b) What is the structure of HCN?

linear

c) HCN has a permanent molecular dipole moment of 5.1 D. Estimate the partial charge on each atom. Clearly state any assumptions you make to get your solution.

estimate $r(C\equiv N) = 1.1\,\mathring{A}$

$$\delta = \frac{(0.2082\ \mathring{A}/D)\mu}{r} = \frac{(0.2082\ \mathring{A}/D)(5.1D)}{1.1\mathring{A}} = 0.97 \Rightarrow 97\%\ \text{ionic character}$$

assume partial charge is evenly split between N and C+H

$\Rightarrow \delta = -0.97$ on N, $\delta = +0.48$ on C, $\delta = +0.48$ on H

d) HCN reacts with water vapor and is completely deprotonated according to the following reaction:

$$HCN + H_2O \rightarrow CN^- + H_3O^+$$

Draw the Lewis dot structure of CN^-. Clearly indicate the number of bonds between each atom and the position of any lone electron pairs.

$$\left[\overset{-1}{:C}\equiv\overset{0}{N}:\right]^-$$

e) What is the structure of CN^-?

Still linear

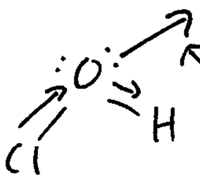
f) CN^- is a vapor at room temperature and is extremely toxic if inhaled. Provide a hypothesis to explain this toxicity.

Because CN^- is diatomic w/ lone pairs available for binding, one hypothesis is that CN^- will bind to the same proteins as O_2 in the body and disrupt their functions. This turns out to be mostly true; the important protein that gets disrupted is cytochrome C oxidase in the electron transport chain.

4. (24 points) For each of the following molecules:

i) Draw the Lewis dot structure;
ii) Determine the VSEPR shape of the molecule and draw the correct three-dimensional shape of the molecule;
iii) Determine whether the molecule has a permanent dipole moment. If it does, draw the orientation of the dipole moment on your VSEPR structure.

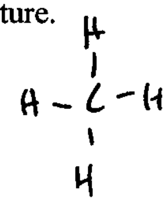
a) OClH

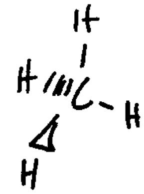


molecular dipole

tetrahedral

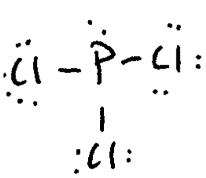
b) CH_4

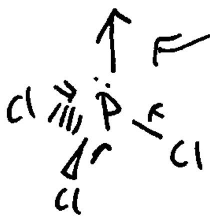




tetrahedral, no dipole

c) PCl_3

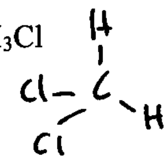


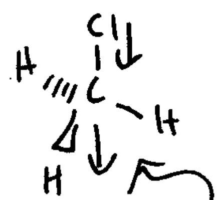


molecular dipole

tetrahedral

d) CH_3Cl

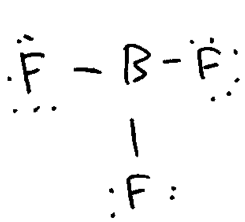


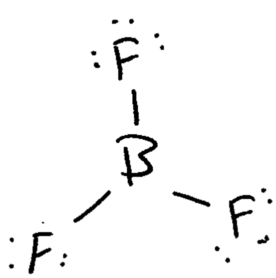


molecular dipole

tetrahedral

e) BF_3





trigonal planar

no dipole

f) BrO_4^-

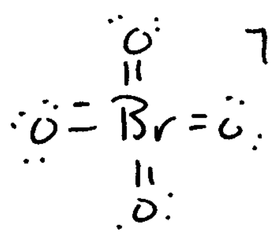
$Br = 7e^-$

$4 \times O = 24e^-$

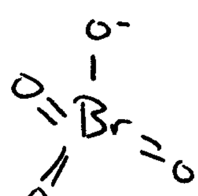
$1e^- = 1e^-$

$32e^-$

7-1



⟷ resonance structures!



tetrahedral, no dipole

5. (20 points) Determine the bond dissociation energy (ΔE_d) of KCl, which has an equilibrium bond length of 2.42 Å.

$\Rightarrow$ $K + Cl \rightarrow KCl$

First we have to ionise K and Cl

(1) $K \longrightarrow K^+ + e^-$ $\quad IE_1 = \frac{4.34\ eV}{atom} \left| \frac{1.602\times10^{-19}\ J}{1\ eV} \right.$

$IE_1 = \frac{6.953\times10^{-19}\ J}{atom} \left| \frac{6.022\times10^{23}\ atoms}{1\ mole} \right.$

$IE_1 = 4.19\times10^5\ J/mol$

(2) $Cl + e^- \longrightarrow Cl^-$ $\quad EA = -349\ KJ/mol$

$= -3.49\times10^5\ J/mol$

Put this together to get energy required to make ions

$V_\infty = IE_1 + EA = 4.19\times10^5\ J/mol - 3.49\times10^5\ J/mol$

$= 0.70\times10^5\ J/mol$

$$V_{bond} = \frac{q_1 q_2}{4\pi\varepsilon_0 r}$$

$$= \frac{(+1)(-1)(1.602\times10^{-19}\ C)^2}{4\times\pi\times(8.854\times10^{-12}\ C^2/Jm)(2.42\times10^{-10}\ m)}$$

$$= -9.5363\times10^{-19}\ J/atom\ (6.022\times10^{23}\ atom/mole)$$

$$= -5.74\times10^5\ J/mol$$

$V_{total} = \Delta E_d = V_\infty + V_{bond} = 0.70\times10^5\ J/mol - 5.74\times10^5\ J/mol$

$= -5.04\times10^5\ J/mol$

$$\boxed{\therefore\ \Delta E_d = -504\ KJ/mol}$$