1st midterm SOLUTIONS

1. (20 points) Xenon tetrafluoride (XeF_4) reacts with water to give atomic xenon (Xe), molecular oxygen (O_2) and HF. How much XeF_4 is needed to give 24.2g of HF?

$$XeF_4 + 2H_2O \longrightarrow Xe + O_2 + 4HF$$

$$MW_{HF} = \underbrace{(1.01 + 19.00)}_{20.01} g/mole, \quad MW_{XeF_4} = \underbrace{[131.3 + 4(19.0)]}_{207.3} g/mole$$

$$\frac{24.2 g\ HF}{20.01\ g HF/mole HF} = 1.21 \text{ moles } HF$$

$$\Rightarrow \underbrace{\tfrac{1}{4}(1.21)}_{0.303} \text{ moles } XeF_4$$

$$= 0.303 \text{ moles } XeF_4 \times \frac{207.3\ g\ XeF_4}{mole\ XeF_4}$$

$$= 62.82\ g\ XeF_4$$

2. (45 points) The two elements X and Y form a diatomic molecule XY with equilibrium bond length 2.37Å. The ionization energies of X and Y are 403 kJ/mole and 1251 kJ/mole, respectively; their electron affinities are 46.9 kJ/mole and 349.0 kJ/mole. Suppose the % ionic character of the XY molecule is 72%, i.e., 0.72e of charge is transferred from one atom to the other when they form the diatomic bond XY.
(a) (15 pts) Which atom ends up negatively charged in the diatomic? Why?

$$(IE + EA)_X = 403 \frac{kJ}{mole} + 46.9 \frac{kJ}{mole} = 449.9 \frac{kJ}{mole}$$

$$(IE + EA)_Y = 1251 \frac{kJ}{mole} + 349.0 \frac{kJ}{mole} = 1600 \frac{kJ}{mole}$$

$$(IE + EA)_X < (IE + EA)_Y \Rightarrow EN_X < EN_Y$$

Thus X gives up electronic charge to Y,

$\Rightarrow$ 'ing Y ends up as negative ion

ALTERNATIVELY,

$(IE_X - EA_Y) < (IE_Y - EA_X) \Rightarrow$ X gives up e to Y

(b) (20 pts) From Coulomb's law and the above information, calculate the bond energy of XY, assuming that a *full* unit of charge (e) is transferred to create atomic ions and an ionic bond.

$$X \rightarrow X^+ + e^- \qquad \Delta E_1 = IE_X$$

$$Y + e^- \rightarrow Y^- \qquad \Delta E_2 = -EA_Y$$

$$X^+ + Y^- \rightarrow XY \qquad \Delta E_3 = \frac{q_{X^+} q_{Y^-}}{4\pi\varepsilon_0 R_e} = \frac{(+e)(-e)}{4\pi\varepsilon_0 R_e}$$

$$X + Y \rightarrow XY \qquad \Delta E = \Delta E_1 + \Delta E_2 + \Delta E_3$$

$$\text{bond energy} = -\Delta E = \frac{e^2}{4\pi\varepsilon_0 R_e} - (IE_X - EA_Y)$$

$$= \frac{(1.602\times10^{-19}\,C)^2}{4\pi(8.854\times10^{-12}\,C^2 J^{-1} m^{-1})(2.37\times10^{-10}\,m)} - (403-349)\frac{kJ}{mole}\,\frac{1\ mole}{6.02\times10^{23}}\,\frac{10^3\,J}{kJ}$$

$$= 9.738\times10^{-19}\,J - 0.897\times10^{-19}\,J = 8.841\times10^{-19}\,J$$

(c) (10 pts) Using the $\mu = QR$ (here Q is the *actual* [i.e., fractional] amount of charge separated, and *R* is the distance between separated charge), calculate the dipole moment of the XY molecule.

$$Q = 0.72e, \qquad R = R_e = 2.37\times10^{-10}\,m$$

$$\mu = QR = (0.72)(1.602\times10^{-19}\,C)(2.37\times10^{-10}\,m)$$

$$= 2.73\times10^{-29}\,C\,m$$

$$= \frac{2.73\times10^{-29}\,C\,m}{0.334\times10^{-29}\,C\,m/D}$$

$$= 8.18\ D$$

3. (20 points) In class and in homework problems, we have been using the simple *Zeff* model

$$Z_{eff} = Z - \begin{pmatrix} \text{number of e's} \\ \text{in lower shells} \end{pmatrix} - \frac{1}{2}\begin{pmatrix} \text{number of other e's} \\ \text{in the same shell} \end{pmatrix},$$

for each electron in a many-electron atom with nuclear charge Ze.

To estimate ionization energies for different atomic species, we used this Zeff in the classical potential energy expression $V = -\frac{Z_{eff}e^2}{4\pi\varepsilon_o r}$.

But now we know that $E_n = -R\frac{Z^2}{n^2}$, *n*= 1, 2, 3, ... , gives the *exact* allowed energies of an electron in the *n*th state of a single-electron atom with atomic number Z. [Here ~~*R* is the~~ Rydberg constant (R=13.6ev).] So now we can use the above model for *Zeff* in the exact expression for *En* to estimate binding energies of electrons in the ground state of a ~~single~~ many-electron atom with atomic number *Z*.

More explicitly, estimate in this way the first ionization energies of He and Li, relative to that of H.

$IE_H = |E_1^H| = R$ ($Z = 1$)

He: 1) The 2 electrons are in the 1st shell (n=1)

2) $Z_{eff} = 2 - 0 - \frac{1}{2}(1) = 3/2$ ($2 = Z_{He}$)

Thus $IE_{He} = \left| -R\frac{Z_{eff}^2}{1^2} \right| = (3/2)^2 R$

and $\frac{IE_{He}}{IE_H} = \frac{9/4\, R}{R} = 9/4$

Li: 1) The 3rd electron, in 2nd shell (n=2) is ionized

2) $Z_{eff} = 3 - 2 - \frac{1}{2}(0) = 1$ ($3 = Z_{Li}$)

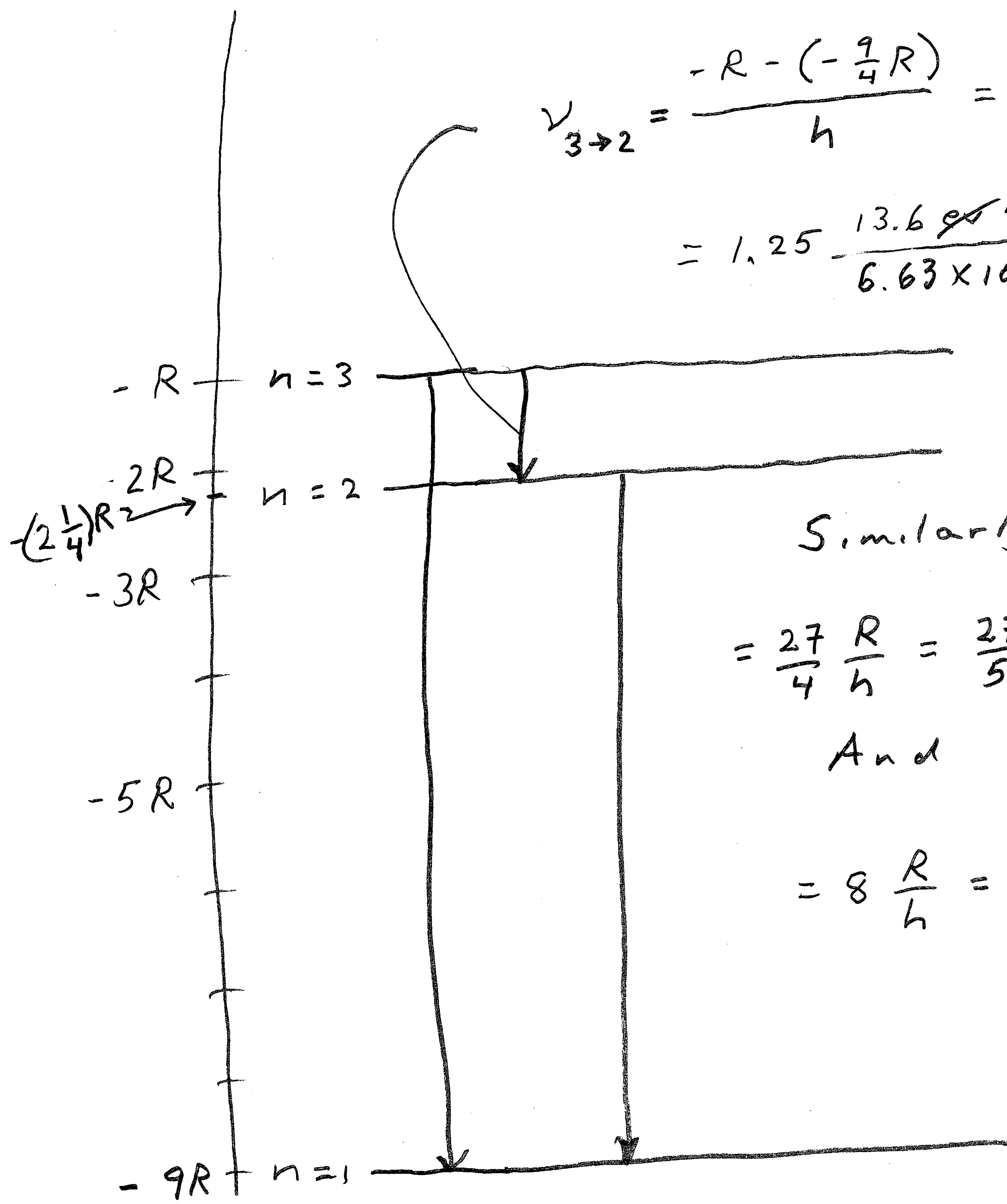
Thus $IE_{Li} = \left| -R\frac{Z_{eff}^2}{2^2} \right| = (1/2)^2 R$

and $\frac{IE_{Li}}{IE_H} = \frac{1/4 \cdot R}{R} = 1/4$

4. (15 points) When Li^{++} is excited to its n=3 state, what are the emission frequencies observed as the ion radiates light to return to its n=2 and n=1 states?

$$E_n = -R\frac{Z^2}{n^2} = -R\frac{9}{n^2} \quad \text{for } Li^{2+}$$

$$= -9R, \quad -\frac{9}{4}R, \quad -R, \ldots$$
$$\quad E_1 \qquad\quad E_2 \qquad\quad E_3$$



$$\nu_{3\to 2} = \frac{-R-(-\frac{9}{4}R)}{h} = +\frac{5}{4}\frac{R}{h}$$

$$= 1.25\,\frac{13.6\ \text{eV}\ 1.602\times10^{-19}\ \text{J/eV}}{6.63\times10^{-34}\ \text{J}\,\text{s}}$$

$$= 4.11\times10^{15}\ s^{-1}$$

$$\text{Similarly, } \nu_{2\to 1} = \frac{-\frac{9}{4}R-(-9R)}{h}$$

$$= \frac{27}{4}\frac{R}{h} = \frac{27}{5}\nu_{3\to 2} = 22.2\times10^{15}\ s^{-1}$$

$$\text{And } \nu_{3\to 1} = \frac{-R-(-9R)}{h}$$

$$= 8\frac{R}{h} = \frac{32}{5}\nu_{3\to 2} = 26.3\times10^{15}\ s^{-1}$$

PERIODIC TABLE (or, at least, the first 54 elements of it...)

Key

11 — Atomic number
Na — Element symbol
Sodium — Element name
22.99 — Average atomic mass*

	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	
1 **H** Hydrogen 1.01																	2 **He** Helium 4.00
3 **Li** Lithium 6.94	4 **Be** Beryllium 9.01											5 **B** Boron 10.81	6 **C** Carbon 12.01	7 **N** Nitrogen 14.01	8 **O** Oxygen 16.00	9 **F** Fluorine 19.00	10 **Ne** Neon 20.18
11 **Na** Sodium 22.99	12 **Mg** Magnesium 24.31											13 **Al** Aluminum 26.98	14 **Si** Silicon 28.09	15 **P** Phosphorus 30.97	16 **S** Sulfur 32.07	17 **Cl** Chlorine 35.45	18 **Ar** Argon 39.95
19 **K** Potassium 39.10	20 **Ca** Calcium 40.08	21 **Sc** Scandium 44.96	22 **Ti** Titanium 47.87	23 **V** Vanadium 50.94	24 **Cr** Chromium 52.00	25 **Mn** Manganese 54.94	26 **Fe** Iron 55.85	27 **Co** Cobalt 58.93	28 **Ni** Nickel 58.69	29 **Cu** Copper 63.55	30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.72	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.92	34 **Se** Selenium 78.96	35 **Br** Bromine 79.90	36 **Kr** Krypton 83.80
37 **Rb** Rubidium 85.47	38 **Sr** Strontium 87.62	39 **Y** Yttrium 88.91	40 **Zr** Zirconium 91.22	41 **Nb** Niobium 92.91	42 **Mo** Molybdenum 95.94	43 **Tc** Technetium (98)	44 **Ru** Ruthenium 101.07	45 **Rh** Rhodium 102.91	46 **Pd** Palladium 106.42	47 **Ag** Silver 107.87	48 **Cd** Cadmium 112.41	49 **In** Indium 114.82	50 **Sn** Tin 118.71	51 **Sb** Antimony 121.76	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90	54 **Xe** Xenon 131.29

$N_{Avogadro}$= 6.02 x 10^{23}/mole

1 ev = 1.602 x 10^{-19} Joule (J)

1 kJ = 10^3 J

1 Debye (D) = 3.336 x 10^{-30} C m

e = 1.602 x 10^{-19} C

1Å= 10^{-10}m

ε_o = 8.854 x 10^{-12} C^2 J^{-1} m^{-1}

h = 6.63 x 10^{-34} J s

$$\upsilon = \frac{c}{\lambda}$$

$E = h\nu$, for energy carried by light of frequency ν

$$V = \frac{q_1 q_2}{4\pi\varepsilon_o r}$$ is the potential energy of two charges interacting at a distance r

R = 13.6 ev

Chem 20A-1

1st MIDTERM, October 23, 2012

NAME________________________________

DISCUSSION SECTION________________

Problem	Points possible	Points scored
1	20	
2(a)	15	
2(b)	20	
2(c)	10	
3	20	
4	15	
	100	

BE SURE TO SHOW ALL YOUR WORK, I.E., MAKE CLEAR THE REASONING BEHIND YOUR SOLUTION TO EACH PROBLEM.

BE CAREFUL TO WRITE UNITS FOR EVERY QUANTITY WITH DIMENSIONS, WITHOUT EXCEPTION.

A PERIODIC TABLE, A LIST OF FUNDAMENTAL CONSTANTS, AND SOME POSSIBLY USEFUL EQUATIONS, ARE PROVIDED ON THE LAST PAGE OF THE EXAM.