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Discussion Section CC2 1D

Midterm #1 (100 pts total + 10 points *extra credit*) **Chem 20A, Winter 2016**

Feburary 5, 2016 (11:00 - 11:50 a.m.)

This exam is closed book but you are allowed one 8.5" x 11" sheet of notes. Non-programmable calculators are allowed, but laptop computers, pocket PC's, palm pilots, etc., are not. Please read the questions carefully and make sure you answer all (and only!) the questions that are asked and be sure that your answers in the appropriate units with a reasonable number of significant figures. Be sure to show all your work as explicitly as possible if you want to receive partial credit, and circle or box your final answer(s); significant figures an units are an important part of each answer. Remember, a correct sentence or two explaining your reasoning and choice of equations will earn most of the points for a problem even if there is a numerical error. (Conversely, incorrect reasoning with a correct answer will result in points being deducted.) If you need additional space, use the back of the page and indicate on the front of the page that your work is continued on the back.

CONSTANTS:

$N_{Av} = 6.0223 \times 10^{23}$ atoms/mole

$e = 1.6022 \times 10^{-19}$ C

$\varepsilon_0 = 8.8542 \times 10^{-12}$ C^2/(J m)

$h = 6.6261 \times 10^{-34}$ J s $= 2\pi\hbar$

$c = 2.9979 \times 10^{8}$ m/s

$m_e = 9.1094 \times 10^{-31}$ kg

$m_p = 1.6726 \times 10^{-27}$ kg

$g = 9.8067$ m/s^2

$\pi = 3.14159$

$k = 1/(4\pi\varepsilon_0) = 8.9875 \times 10^{9}$ (J m)/C^2

Atomic weight of Fe = 55.847 g/mole

CONVERSION FACTORS:

1 atomic mass unit = 1.6605×10^{-27} kg

1 eV = 1.602×10^{-19} J = 96.485 kJ/mole

1 Å = 1×10^{-10} m

1 kJ = 1000 J

FORMULAS:

$E_{ph} = h\nu = hc/\lambda$

K.E. = $1/2\, m\, v^2$ with $v = |v| = (v_x^2 + v_y^2 + v_z^2)^{1/2}$

deBroglie Wavelength: $\lambda = h/p\, ;\, p = mv$

$F = -\Delta U/\Delta x$

Coulomb Potential: $U(r) = q_1 q_2/(4\pi\varepsilon_0 r)$

Coulomb Force: $F_C = q_1 q_2/(4\pi\varepsilon_0 r^2)$

Bragg Formula for maxima: $n\lambda = d \sin\theta$

One-electron Energy Levels: $$E = -\frac{me^4Z^2}{2h^2(4\pi\varepsilon_0)^2n^2} = -R_\infty\frac{Z^2}{n^2} = -(13.6\text{ eV})\frac{Z^2}{n^2}$$

#1	41
#2	25
#3	25
Total	91

This exam has 7 total pages, including this cover page

Midterm (Continued) **Chem 20A, Winter 2016**

3. (Continued)

We know from our discussion of radial distribution functions that there is a small but non-zero probability that an electron in a $3p$ orbital can be found closer to the nucleus than electrons in lower shells. Using values from the table on the previous page, calculate both how well a $3p$ electron (with two $3s$ but no $3d$ or any $n = 4$ or higher-shell electrons present) screens the nucleus from a $2s$ electron, and how well a $3p$ electron screens the nucleus from a $1s$ electron. In other words, how does the Z_{eff} for a $1s$ or $2s$ electron change when an atom gains a single $3p$ electron? Be sure to make clear which values you've taken from the table and why you chose those particular values. Note: No credit will be given for using the crude Z_{eff} model discussed in the lecture.

⇒ We work from w/ e configuration – $1s^2 2s^2 2p^6 3s^2$ – Mg
Gain 3p e⁻ – $1s^2 2s^2 2p^6 3s^2 3p^1$ – Al.

1s electron in ~~Mg~~ goes from 11.619 in Mg to 12.591 in Al.

Expected Zeff to increase by 1 but it instead increased by .972.
We can conclude that 3p electron screens the 1s electron by 1 – .972 = .028, which is relatively insignificant

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2s electron in ~~Mg~~ goes from Zeff of ~~11.619~~ 7.392 in Mg to 8.214 in Al.

Expected Zeff to increase by 1, but instead it increased by .822. We conclude that the 3p electron in Al screens ~~2p~~ electron by .178.

+25

Name___________________________

Midterm (Continued) **Chem 20A, Winter 2016**

1. (45 pts total). A KrF excimer laser can produce pulses of light in the ultraviolet region of the spectrum with a wavelength of 248 nm and a total pulse energy of 0.250 J. If one of these laser pulses is focused onto the surface of Cs metal (whose work function is 3.43×10^{-19} J, as we discussed in class), electrons are ejected.

(a) (10 pts) How many electrons are ejected from the Cs metal per laser pulse?

6

$E_{photon} = \frac{hc}{\lambda} = 8.0098 \times 10^{-19}$ J $> 3.43 \times 10^{-19}$ J

so electrons are ejected!

$\frac{.25 \text{ J}}{3.43 \times 10^{-19} \text{ J}} = 3.121176 \times 10^{17}$ photons.

-1 #N

Each electron is energized by 1 photon, so total # of electrons ejected =

-1 3.121176×10^{17} electrons

9 (b) (10 pts) What is the kinetic energy of each of the ejected electrons?

$E_{photon} = hf = \frac{hc}{\lambda} = 8.0098 \times 10^{-19}$ J

-1

$K_{electron} = E_{photon} - E_{wf} = 4.5798378 \times 10^{-19}$ J

$\frac{1}{2} m_e V_e^2 = K_{electron}$

$V_e = 1002755$ m/s

-1 (same sig figs)

17

Name________________________

Midterm (Continued) **Chem 20A, Winter 2016**

1. (Continued)

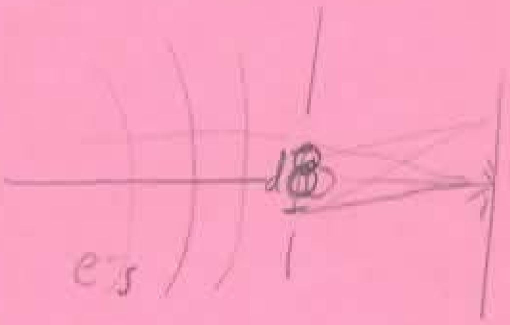
(c) (5 pts) If Oxygen atoms, which have an electron affinity of 2.35×10^{-19} J are present in the space above the Cs metal, can the O atoms capture the ejected electrons to form O^- ions? Why or why not?

5

No. e- affinity is less than the energy required to eject an electron from the cesium atom.

(d) (20 pts) Suppose the electrons that are ejected from the Cs metal are collimated into a beam which is then used in an electron microscope. The electron beam impinges on a large diatomic molecule, which behaves as two "slits" spaced a distance *d* apart. On a screen behind the beam, a bright spot appears at "zero" degrees because part of the beam goes straight past the molecule and hits the screen. The angular separation between this bright spot and the next closest bright spot is 47.2 degrees. Calculate the bond length (distance between "slits") of the diatomic molecule.

14



$n(\lambda) = d\sin\theta$

$d = \frac{n\lambda}{\sin\theta}$

$\lambda_{e^-} = \frac{h}{mv} = 7.2539 \times 10^{-10}$ m

$\frac{n(\lambda_{e^-})}{\sin\theta}$

$d = 9.8868 \times 10^{-10}$ m $= \frac{(2-1)(\lambda_{e^-})}{\sin\theta}$

24

Midterm (Continued) **Chem 20A, Winter 2016**

2. (30 pts total) The blood of mammals contains a large iron-containing molecule called hemoglobin (Hb). The Fe atoms in Hb formally have a +2 charge. When the blood is circulated near the lungs, each iron atom in the Hb can bind (react) with an oxygen molecule to form oxygenated hemoglobin (O_2:Hb). The blood is then circulated throughout the body and the bound oxygen molecules are released by the Hb where needed. Carbon monoxide (CO) or cyanide (CN^-) poisoning is deadly because CO molecules and CN^- anions can also bind to the Fe^{2+} atoms in Hb. When CO or CN^- is bound to the Fe^{2+} in Hb, the Hb molecule can no longer bind O_2 and thus the blood can no longer efficiently transport oxygen throughout the body.

   (a) (20 pts) It is known from many experiments that the Hb molecule contains 0.335% by weight Fe atoms, and that there are 4 Fe atoms per Hb molecule. What is the molecular weight of Hb?

4 mols Fe ~~4 Fe atoms~~ → 4 · 55.933 g/mol = 223.732 g

~~4 Fe atoms~~.

(223.732 g 4Fe) = .(.00335)(molar mass Hb)

66785.67 g/mol (molar weight of Hb) 20

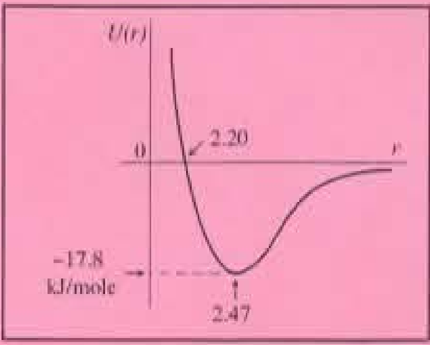
66785.67 g/mol · 1 mol / 6.0223 × 10^23 molecules = 1.10897 × 10^-19 g/molecule

Name________________________

Midterm (Continued) **Chem 20A, Winter 2016**

2. (Continued)

(b) (10 pts) Suppose the interaction between the Fe^{2+} atoms in Hb and either CO or O_2 molecules can be modeled by the potential energy curve shown at right (this type of curve is typical for species which can react to form chemical bonds). If the CO (or O_2) molecule is separated from the Fe atom by its equilibrium distance of 2.47 Å, what is the force (in Newtons) between the CO (or O_2) molecule and the Fe^{2+} atom in Hb? How much energy (in J) does it take to unbind *single* CO (or O_2) molecule from the Fe^{2+} atom in Hb?



$U = \frac{-q \cdot q}{4\pi\varepsilon_0 r}$ $F = \frac{q\,q}{4\pi\varepsilon_0 r^2}$

$F = \frac{-U}{r} = 7.206477 \times 10^{10}$ kN/mole

7.2064×10^{10} kN/mol $\cdot \frac{1000\ N}{1\ kN} \cdot \frac{1\ mol}{6.02 \times 10^{23}\ atoms} = 1.1966 \times 10^{-10}$ N

X

To unbind: 17.8 kJ/mole $\cdot \frac{1000\ J}{1\ kJ} \cdot \frac{1\ mole}{6.02 \times 10^{23}\ atoms}$

~~= 29557 J/~~

$= 2.9557 \times 10^{-20}$ J/single CO (or O_2)

Midterm (Continued) **Chem 20A, Winter 2016**

3. (25 points total) The table below shows the best-known values of Z_{eff} for the electrons in different orbitals in each of the first 36 atoms of the periodic table:

Effective nuclear charges for elements 1 to 36

Z	Element	1s	2s	2p	3s	3p	4s	3d	4p
1	H	1.000							
2	He	1.688							
3	Li	2.691	1.279						
4	Be	3.685	1.912						
5	B	4.680	2.576	2.421					
6	C	5.673	3.217	3.136					
7	N	6.665	3.847	3.834					
8	O	7.658	4.492	4.453					
9	F	8.650	5.128	5.100					
10	Ne	9.642	5.758	5.758					
11	Na	10.626	6.571	6.802	2.507				
12	Mg	11.619	7.392	7.826	3.308				
13	Al	12.591	8.214	8.963	4.117	4.066			
14	Si	13.575	9.020	9.945	4.903	4.285			
15	P	14.558	9.825	10.961	5.642	4.886			
16	S	15.541	10.629	11.977	6.367	5.482			
17	Cl	16.524	11.430	12.993	7.068	6.116			
18	Ar	17.508	12.230	14.008	7.757	6.764			
19	K	18.490	13.006	15.027	8.680	7.726	3.495		
20	Ca	19.473	13.776	16.041	9.602	8.658	4.398		
21	Sc	20.457	14.574	17.055	10.340	9.406	4.632	7.120	
22	Ti	21.441	15.377	18.065	11.033	10.104	4.817	8.141	
23	V	22.426	16.181	19.073	11.709	10.785	4.981	8.983	
24	Cr	23.414	16.984	20.075	12.368	11.466	5.133	9.757	
25	Mn	24.396	17.794	21.084	13.018	12.109	5.283	10.528	
26	Fe	25.381	18.599	22.089	13.676	12.778	5.434	11.180	
27	Co	26.367	19.405	23.092	14.322	13.435	5.576	11.855	
28	Ni	27.353	20.213	24.095	14.961	14.085	5.711	12.530	
29	Cu	28.339	21.020	25.097	15.594	14.731	5.858	13.201	
30	Zn	29.325	21.828	26.098	16.219	15.369	5.965	13.878	
31	Ga	30.309	22.599	27.091	16.996	16.204	7.067	15.093	6.222
32	Ge	31.294	23.365	28.082	17.760	17.014	8.044	16.251	6.780
33	As	32.278	24.127	29.074	18.596	17.850	8.944	17.378	7.449
34	Se	33.262	24.888	30.065	19.403	18.705	9.758	18.477	8.287
35	Br	34.247	25.643	31.056	20.218	19.571	10.553	19.559	9.028
36	Kr	35.232	26.398	32.047	21.033	20.434	11.316	20.626	9.769

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Midterm (Continued) **Chem 20A, Winter 2016**

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