3033036281

Chemistry 4A, Exam II
October 9, 2017
Professor R.J. Saykally

Name Michael Li

GSI Hannah Kenagy

1. (25) __________

2. (15) __________

3. (20) __________

4. (25) __________

5. (15) __________

TOTAL EXAM SCORE (100) __________

Rules:

- Work all problems to 2 significant figures
- No lecture notes or books permitted
- No programmable or graphing calculators permitted
- Time: 50 minutes
- Show all work to get partial credit
- All answers must be written in the boxes provided
- Periodic Table, Tables of Physical Constants, and Conversion Factors included

Periodic Table of the Elements

BERKELEY LAB

WORKFORCE DEVELOPMENT & EDUCATION

Glenn T Seaborg

atomic number	14
atomic weight	28.09
symbol	Si
name	Silicon

symbol: **black** solid
blue liquid
red gas
white synthetically prepared *most stable isotope*
grey synthetically prepared; later found in trace amounts in nature

- alkali metals
- alkaline earth metals
- transition metals
- other metals
- metalloids
- noble gases
- halogens
- other non-metals
- unknown chemical properties
- discovery claimed

1 1.01 H Hydrogen																	2 4.003 He Helium
3 6.94 Li Lithium	[redacted]											5 10.81 B Boron	6 12.01 C Carbon	7 14.01 N Nitrogen	8 15.999 O Oxygen	9 18.998 F Fluorine	10 20.18 Ne Neon
11 22.99 Na Sodium	[redacted]											13 26.98 Al Aluminum	14 28.09 Si Silicon	15 30.97 P Phosphorus	16 32.06 S Sulfur	17 35.45 Cl Chlorine	18 39.95 Ar Argon
19 39.10 K Potassium	[redacted]	21 44.96 Sc Scandium	22 47.90 Ti Titanium	23 50.94 V Vanadium	24 51.996 Cr Chromium	25 54.94 Mn Manganese	26 55.85 Fe Iron	27 58.93 Co Cobalt	28 58.69 Ni Nickel	29 63.55 Cu Copper	30 65.41 Zn Zinc	31 69.72 Ga Gallium	32 72.64 Ge Germanium	33 74.92 As Arsenic	34 78.96 Se Selenium	35 79.90 Br Bromine	36 83.80 Kr Krypton
37 85.47 Rb Rubidium	[redacted]	39 88.91 Y Yttrium	40 91.22 Zr Zirconium	41 92.91 Nb Niobium	42 95.94 Mo Molybdenum	43 (98) Tc*** Technetium	44 101.07 Ru Ruthenium	45 102.91 Rh Rhodium	46 106.42 Pd Palladium	47 107.87 Ag Silver	48 112.41 Cd Cadmium	49 114.82 In Indium	50 118.71 Sn Tin	51 121.76 Sb Antimony	52 127.60 Te Tellurium	53 126.90 I Iodine	54 131.29 Xe Xenon
55 132.91 Cs Cesium	[redacted]	57 138.91 La ▸ Lanthanum	72 178.49 Hf Hafnium	73 180.95 Ta Tantalum	74 183.84 W Tungsten	75 186.21 Re Rhenium	76 190.23 Os Osmium	77 192.22 Ir Iridium	78 195.08 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury	81 204.38 Tl Thallium	82 207.2 Pb Lead	83 208.98 Bi Bismuth	84 (209) Po Polonium	85 (210) At* Astatine	86 (222) Rn Radon
87 (223) Fr Francium	[redacted]	89 227.03 Ac ▸▸ Actinium	104 (261) Rf* Rutherfordium	105 (262) Db* Dubnium	106 (266) Sg* Seaborgium	107 (264) Bh Bohrium	108 (277) Hs Hassium	109 (268) Mt Meitnerium	110 (281) Ds Darmstadtium	111 (272) Rg Roentgenium	112 (285) Cn Copernicium	113 — Uut Ununtrium	114 (289) Fl Flerovium	115 — Uup Ununpentium	116 (293) Lv Livermorium	117 — Uus Ununseptium	118 — Uuo Ununoctium

Lanthanide series ▸	58 140.12 Ce Cerium	59 140.91 Pr Praseodymium	60 144.24 Nd Neodymium	61 (145) Pm Promethium	62 150.36 Sm Samarium	63 151.96 Eu Europium	64 157.25 Gd Gadolinium	65 158.93 Tb Terbium	66 162.50 Dy Dysprosium	67 164.93 Ho Holmium	68 167.26 Er Erbium	69 168.93 Tm Thulium	70 173.04 Yb Ytterbium	71 174.97 Lu Lutetium
Actinide series ▸▸	90 232.04 Th Thorium	91 231.04 Pa Protactinium	92 238.03 U Uranium	93 237.05 Np* Neptunium	94 (244) Pu* Plutonium	95 (243) Am** Americium	96 (247) Cm* Curium	97 (247) Bk* Berkelium	98 (251) Cf* Californium	99 (252) Es* Einsteinium	100 (257) Fm* Fermium	101 (258) Md* Mendelevium	102 (259) No* Nobelium	103 (262) Lr* Lawrencium

* Discovered at Lawrence Berkeley National Laboratory
** Discovered in Chicago by Berkeley team
*** Discovered in Italy using a sample from Berkeley cyclotron bombardment

Physical Constants

Standard Acceleration of terrestrial gravity	$g = 9.80665$ m s^{-2} (exactly)
Avogadro's number	$N_0 = 6.022137 \times 10^{23}$
Bohr radius	$a_0 = 0.52917725$ Å $= 5.2917725 \times 10^{-11}$ m
Boltzmann's constant	$k_B = 1.38066 \times 10^{-23}$ J K^{-1}
Electron Charge	$e = 1.6021773 \times 10^{-19}$ C
Faraday constant	$\mathcal{F} = 96{,}485.31$ C mol^{-1}
Masses of fundamental particles:	
Electron	$m_e = 9.109390 \times 10^{-31}$ kg
Proton	$m_p = 1.672623 \times 10^{-27}$ kg
Neutron	$m_n = 1.674929 \times 10^{-27}$ kg
Ratio of proton mass to electron mass	$m_p/m_e = 1836.15270$
Permittivity of vacuum	$\epsilon_0 = 8.8541878 \times 10^{-12}$ C^2 J^{-1} m^{-1}
Planck's constant	$h = 6.626076 \times 10^{-34}$ J s
Speed of light in vacuum	$c = 2.99792458 \times 10^{8}$ m s^{-1} (exactly)
Universal gas Constant	$R = 8.31451$ J mol^{-1} K^{-1} $= 0.0820578$ L atm mol^{-1} K^{-1}

Conversion Factors

Standard Atmosphere	1 atm = 1.01325×10^{5} Pa = 1.01325×10^{5} kg m^{-1} s^{-2} (exactly)
Atomic mass unit	1 u = 1.660540×10^{-27} kg
	1 u = 1.492419×10^{-10} J = 931.4942 MeV (energy equivalent from E = mc2)
Calorie	1 cal = 4.184 J (exactly)
Electron volt	1 eV = $1.6021773 \times 10^{-10}$ J = 96.48531 kJ mol^{-1}
Foot	1 ft = 12 in = 0.3048 m (exactly)
Gallon (U.S.)	1 gallon = 4 quarts = 3.78541 L (exactly)
Liter-atmosphere	1 L atm = 101.325 J (exactly)
Metric ton	1 metric ton = 1000 kg (exactly)
Pound	1 lb = 16 oz = 0.45359237 kg (exactly)

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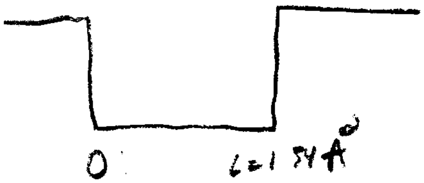
1. (5 points each)

A) Estimate the energy of an electron in a C=C double bond (L = 1.34Å) for its lowest 2 states using a 1-D quantum well model.

For 1-D quantumwell



$E = \frac{n^2h^2}{8m_eL^2}$ $n = 1, 2, 3 \ldots$

$m_e = 9.109390\times10^{-31}$ kg

Lowest State $n=1$

$$E_1 = \frac{1^2(6.626\times10^{-34})^2}{8\cdot 9.109390\times10^{-31}(1.34\times10^{-10})^2} = \boxed{3.4\times10^{-18}\,J}$$

3.35×10^{-18} J

Second Lowest state

$$E_2 = \frac{2^2(6.626\times10^{-34})^2}{8\cdot 9.109390\times10^{-31}\cdot(1.34\times10^{-10})^2} = \boxed{1.3\times10^{-17}\,J}$$

1.342×10^{-17} J

B) Calculate the wavelength of light necessary to excite the electron between these 2 states.

$\Delta E = E_2 - E_1 = h\nu = hc/\lambda$ $n=2 \rightarrow n=1$

E_2 from part A $= 1.3\times10^{-17}$ J E_1 from part A $= 3.4\times10^{-18}$ J

So $\frac{hc}{E_2-E_1} = \lambda$

$$\frac{(6.626\times10^{-34}\,\cancel{J}\cancel{s})(2.998\times10^{8})\,m/\cancel{s}}{(1.3\times10^{-17} - 3.4\times10^{-18})\,\cancel{J}} = 1.9735\times10^{-8}\,m$$

$$= \boxed{2.0\times10^{-8}\,m}$$

C) Calculate the momentum of photon with this wavelength.

$\lambda = \frac{h}{p}$ so $p = \frac{h}{\lambda}$

$$p = \frac{6.626 \times 10^{-34}\,\text{Js}}{(1.97 \times 10^{-8})} = 3.357 \times 10^{-26}\,\text{kgm/s}$$

$$= \boxed{3.3 \times 10^{-26}\,\text{kgm/s}}$$

D) Calculate the uncertainty in position of an electron having this momentum.

$$\underset{\text{uncertainty in } x}{(\sigma_x)}\underset{\text{uncertainty in momentum}}{(\sigma_p)} \geq h/4\pi$$

from part C $p = 3.3 \times 10^{-26}$ kg m/s

$\sigma_x = \frac{h/4\pi}{p}$ so $\sigma_x \geq \frac{6.626 \times 10^{-34}}{4 \cdot \pi \cdot 3.3 \times 10^{-26}}$

$\sigma_x \geq 1.597 \times 10^{-9}$

at least

the uncertainty of position is greater than

$$\boxed{\sigma_x \geq 1.6 \times 10^{-9}\ \text{m}}$$

E) Show (by calculation) that the cos(ax) function is not an acceptable solution to the Schrödinger equation for this problem.

So inorder to hae a particle in a 1-D quantum well, $\psi(0)=0$ and $\psi(L)=0$

so with the cos(ax) function with $\psi = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)$

$x=0$

$\psi(0)$ is equa to $\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi 0}{L}\right) = \sqrt{\frac{2}{L}}$ which is $\neq 0$

$\psi(L)$ is equa to $\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi L}{L}\right) = \pm\sqrt{\frac{2}{L}}$ which is $\neq 0$

Thus cos(ax) function is not an acceptable solution to the schrodinger equation

2. (5 points each) Arrange the following substances in order and explain your choice of order

A) Mg^{2-}, Ar, Br^-, Ca^{2-} in order of increasing radius

Mg^{2+} has outer electrons in the 2p while Ar has outer electrons in the 3p so b/c r ∝ n^2, Ar radius is greater than Mg^{2+}. However, Ca^{2+} is isoelectronic w/ Ar but has higher nuclear charge but has outer electrons in 3p so $Mg^{2+} < Ca^{2+} < Ar$. Br^- has outer electrons in 4p so because n is greater for Br^-, radius of Br^-

$Br^-_{radius} >$ radius Ar

$Mg^{2+} < Ca^{2+} < Ar <$

B) Na, Na^+, O, Ne in order of increasing ionization energy

so Na has outer electrons in 3s which has a higher n than any of the other atoms so it has an electron the furthest from the nucleus and thus has the smallest IE. O, Ne and Na^+ all have electrons in the 2p but O has the smallest Z_{eff} and Ne has the second smallest Z_{eff} so IE O will the smallest as those outer electrons feel less electrostatic attraction towards its nucleus. So, it'll easier to ionize. By the same trend $IE_O < IE_{Ne} < IE_{Na^+}$

$Na < O < Ne < Na^+$

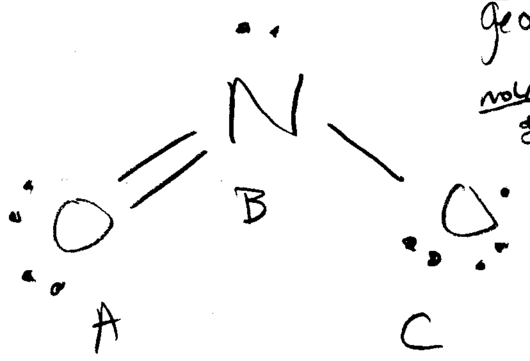
C) H, F, Al, O in order of increasing electronegativity

Al is a metal so it wants to form positive complexes so it has the lowest EN. Hydrogen is second lowest as it has no desire to fill its 1s and it would create excess $e^- - e^-$ repulsion, O has the second highest as F would try and get another electron to make it have filled shell stability so,

$Al < H < O < F$

3. (5 points each) Consider the bonding in the NO_2 molecule.

A) Use VSEPR to determine the geometry (sketch and label) and hybridization.

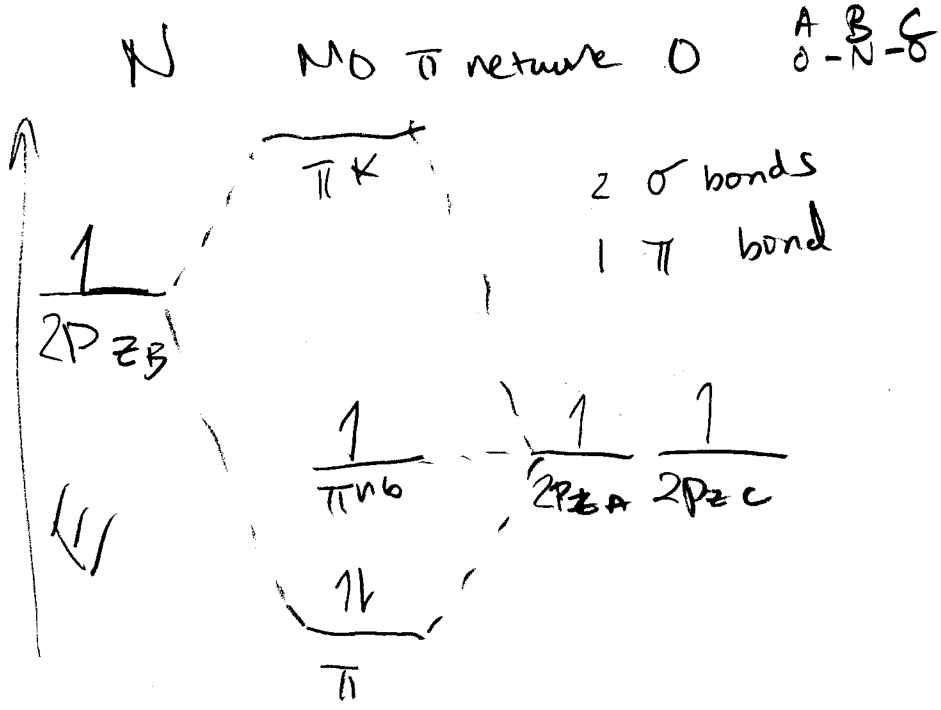


electronic geometry = trigonal planar

molecular geometry = bent

hybridization = sp^2

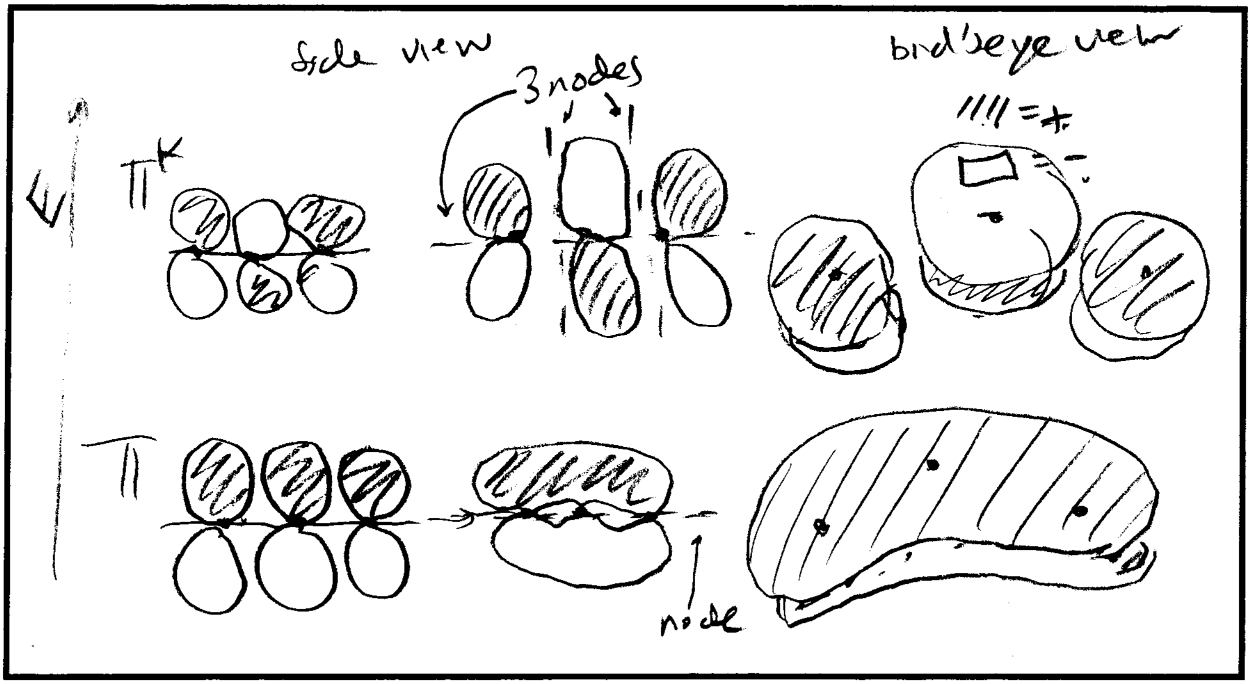
B) Draw the correlation diagram for the pi molecular orbitals (using the convention of your text), showing the occupancy. Specify the number of sigma and pi bonds.



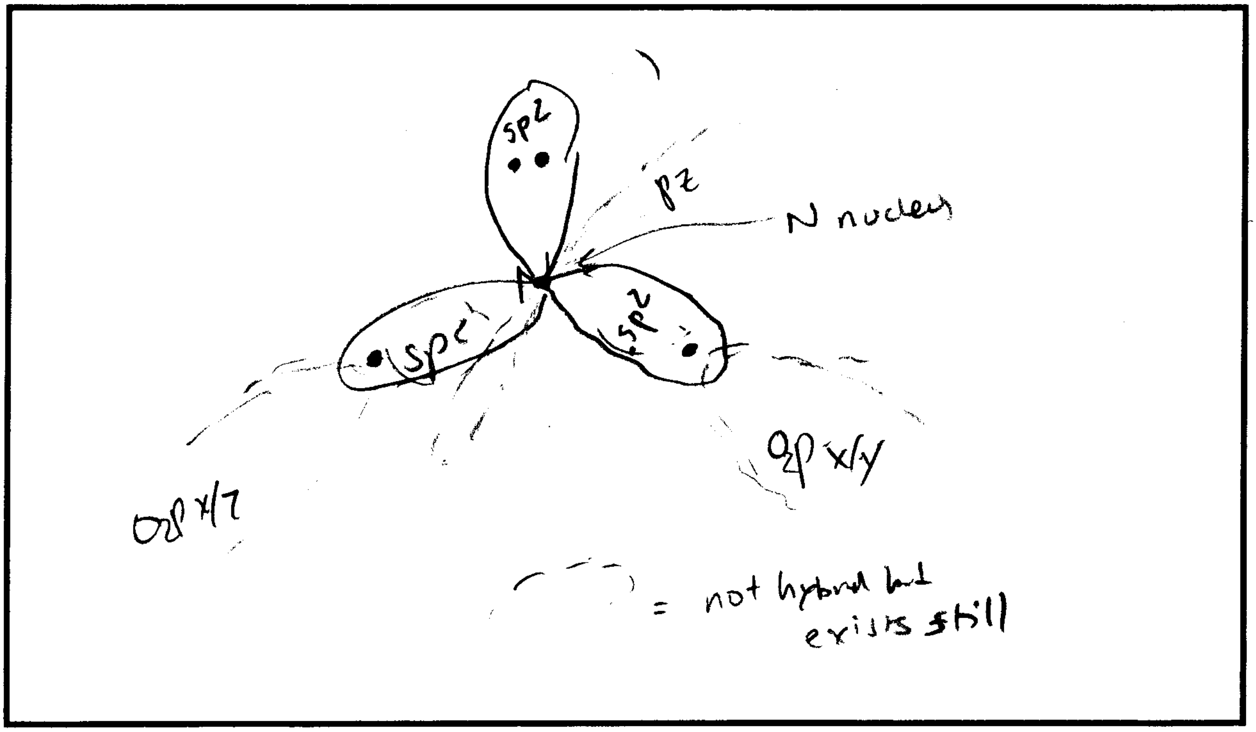
2 σ bonds

1 π bond

C) Sketch the shapes of the π and π^* molecular orbitals, labeling the axes and nodes.



D) Sketch all the hybrid orbitals localized on the nitrogen.



4. (5 points each) If an electron is removed from a nitrogen (N_2) molecule, an N_2^+ molecular ion forms:

A) Give the molecular electron configurations for N_2 and N_2^+.

N_2 : $(\sigma_{1s})^2 (\sigma^*_{1s})^2 (\sigma_{2pz})^2 (\pi_{2px}, \pi_{2py})^4$

N_2^+. $(\sigma_{1s})^2 (\sigma^*_{1s})^2 (\sigma_{2pz})^2 (\pi_{2px}, \pi_{2py})^3$

B) Give the bond order of each species

$BO_{N_2} = \frac{1}{2}(8-2) = \frac{1}{2} \cdot 6 = \boxed{3} = BO_{N_2}$ $BO = \frac{1}{2}$(bonding e^- - antibonding e^-)

$BO_{N_2^+} = \frac{1}{2}(7-2) = \frac{1}{2} \cdot 5 = \boxed{2\frac{1}{2}} = BO_{N_2^+}$

$\frac{5}{2}$ "

C) Predict which species should be paramagnetic.

$\boxed{N_2^+}$ is predicted to be paramagnetic as it has an unpaired electron in one of the (π_{2px}) or (π_{2py}) orbitals

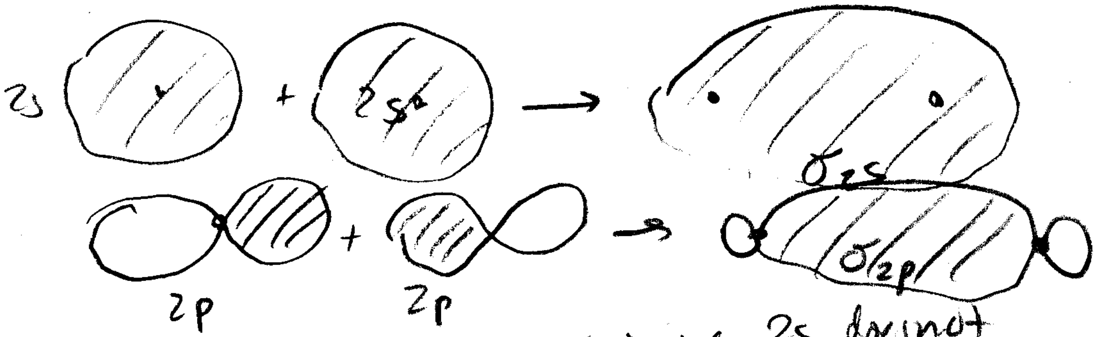
D) Predict which species has the greater bond dissociation energy

Because BO $N_2 = 3 > 2.5 = BO_{N_2^+}$,

$\boxed{N_2}$ will be predicted to have a greater bond dissociation energy

3 > 2.5

E) Why is a σ (2s) orbital lower in energy than a σ (2p) orbital in a homonuclear diatomic?



σ 2p has nodes on the nuclei while 2s does not, destructively interfere very slightly to
Also, 2p has two lobes which create a lower electron density inbetween the two nuclei. Both these reasons cause σ_{2p} to be less favorable than σ_{2s} for bonding which makes $E\sigma_{2p} > E\sigma_{2s}$ and also $E\sigma_{2s}$ will be lower in energy (more stable) than σ_{2p}

5. (5 points each) The wave function of an electron in the lowest (that is, ground) state of the hydrogen atom is

$$\Psi(\mathrm{r}) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} \exp\left(\frac{-r}{a_0}\right)$$

$$a_0 = 0.529 \times 10^{-10}\mathrm{m}$$

A) Write the integral that you would use to determine the probability of finding the electron inside a sphere of volume 1.0 pm^3, centered at the nucleus (1 pm = 10^{-12} m)? You do not need to evaluate the integral.

$1.0 pm^3 \cdot \left(\frac{10^{-12} m}{1 pm}\right)^3 = 1.0 \times 10^{-36} m^3 = \frac{4}{3}\pi r^3$

probability = $\int |\psi(r)|^2 dr$ $\quad r = \sqrt[3]{\frac{3}{4\pi} \cdot 1.0\times 10^{-36}}$

$|\psi(r)|^2 = \left(\frac{1}{\pi a_0^3}\right) e^{-2r/a_0} dr$ $\quad r = 6.2035 \times 10^{-13} m$

$$\boxed{\text{probability} = \int_{r=0}^{r=6.2035\times 10^{-13} m} \frac{1}{\pi a_0^3} \cdot e^{-2r/a_0} dr}$$

B) Calculate the wavelength necessary to break the bond in the H_2 molecule (D_e = 431 kJ/mol).

$$De = 431\,kJ/mol \times \frac{1\,mole}{6.023\times10^{23}\,molecule} \times \frac{1000J}{1kJ}$$

$$= 7.156\times10^{-19}\ J/molecule$$

for 1 molecule H_2, you need $7.156\times10^{-19}J$ energy

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

$$\text{so } \lambda = \left(\frac{6.626\times10^{-34}\times 3\times10^{8}}{7.156\times10^{-19}}\right) = 2.7778\times10^{-7}m$$

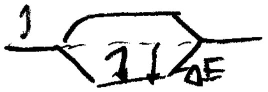
$$= \boxed{2.8\times10^{-7}m}$$

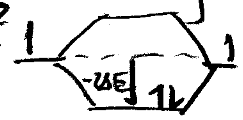
C) Estimate the bond energy for the H_2^+ ion.

H_2^+ molecular electron configuration $= (\sigma_{1s})^1$

H_2 molecular electron config $= (\sigma_{1s})^2$

$BO_{H_2^+} = 1/2$





$BO_{H_2} = 1$

so $\text{Bond Energy}_{H_2^+} = -\Delta E$

$BE_{H_2} = -2\Delta E$

$-2\Delta E = 431\,kJ/mol$

$\Delta E = -215\,kJ/mol$

$\text{Bondenergy}_{H_2^+} = \boxed{215\,kJ/mol}$ ⇒ Bond dissociation Energy = amount of energy to break to bond = 215 kJ/mol