Full Name: _____ **Seat Number:** _____

Student Number: _____

CHM 2311
Midterm 1
February 26, 2009
Professor Darrin Richeson

You have 80 minutes to complete this exam.
Please read the questions carefully.
There some useful equations and a periodic table on the last 2 pages of the exam.

Please write legibly and show your work to receive credit for your answers.
Partial marks *may in some cases* **be awarded for partially correct work.**

Question	Mark		Question	Mark
1	**/ 10**		**6**	**/ 2**
2	**/ 6**		**7**	**/ 5**
3	**/ 5**		**8**	**/ 12**
4	**/ 3**		**9**	**/ 8**
5	**/ 3**		**10**	**/ 6**
Total				**/60**

1. **(10 points) In class, we looked at a one-dimensional particle in a box with infinite potential energy walls and length of *a.***
(a) A ground state electron in a one-dimensional box absorbs 1480 nm light. The box has a length of 1.34 nm. What is the value of n for this excited particle?

First notice that this is a particle in a box not a hydrogen atom. We do not use the Balmer equation!
Also note that the ground state of the electron is n = 1

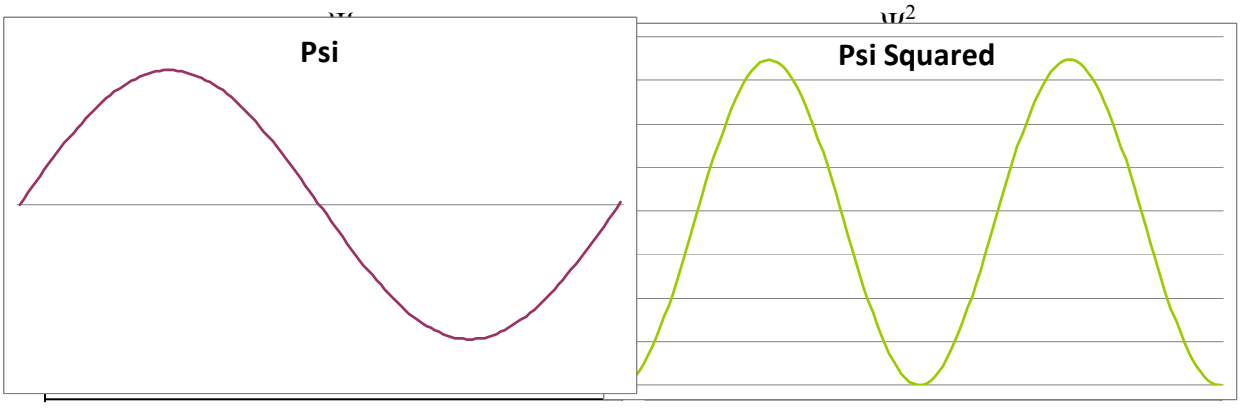
Energy of 1480 nm light using $E = h\nu = hc/\lambda = 6.626 \times 10^{-34} Js\ (3 \times 10^{8}\ m/s)/1480 \times 10^{-9}\ m$

$E = 1.34 \times 10^{-19}\ J$ *This value corresponds to the energy difference between the n = 1 and n state*
Now we need to calculate the value of n using this energy:

$$n^2 = \frac{E8ma^2}{h^2} = \frac{(1.34\times10^{-19}\,J)(8)(9.11\times10^{-31}\,kg)(1.34\times10^{-9}\,m)^2}{(6.626\times10^{-34}\,J\bullet s)^2}$$

$n^2 = 4.0$
$n = 2$

(b) Sketch the wave function, ψ, and the probability function, ψ^2, for the quantum level, n, found in part (a) above.



(c) What value(s) of x correspond to a minimum probability for the electron?
At the values 0 and a
Also at the value a/2

2. **(6 points)** After the particle in a box, we moved to solutions of the Schrödinger equation in three dimensions and obtained 3 quantum numbers.

What are their symbols and possible values?

Quantum number	Possible Values
n	Integers beginning at 1
l	0, 1, 2…n-1
m_l	*-l*….0….*+l*

3. **(5 points)** The angular portion of a hydrogen orbital can be expressed in either Cartesian or polar coordinates. An example of an angular wave function is given by:

Cartesian coordinates $$Y(x,y,z) = \sqrt{\frac{15}{4\pi}}\frac{xz}{r^2}$$

(a).Which planes (a plane being defined by two of the three coordinates x, y or z) correspond to nodes for this orbital?

Zero values are obtained for x = 0 and any values of z or y
or *z = 0 and any value of x and y.*

This is equivalent to saying that there are nodes for the ***xy plane*** *(perpendicular to the z axis) and for the* ***yz plane*** *(perpendicular to the x axis).*

(b) If this same orbital has 1 ***radial*** node, identify the orbital using the conventional label (e.g. 2s, $4p_x$, $3d_{z^2}$, etc.) and ***show the thought process*** by which you were able to reach your answer.

This orbital has two angular nodes and is therefore a d orbital. More specifically it is the d_{xz} *orbital. The fact that there is one radial node indicates that it is the* $4d_{xz}$*.*

4. **(3 points)** Calculate Z_{eff} for an electron in the 4p orbital of the Sn atom.

Electronic configuration of Sn [Kr] $5s^2 4d^{10} 5p^2$ = [$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$] $5s^2 4d^{10} 5p^2$

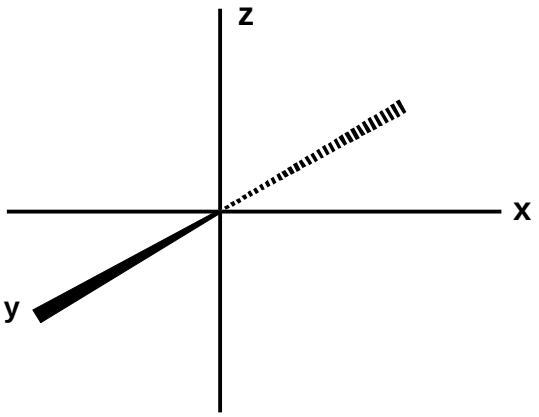
*($1s^2$)($2s^2 2p^6$)($3s^2 3p^6$)($3d^{10}$) ($4s^2$ **$4p^6$**)($4d^{10}$)($5s^2 5p^2$)*

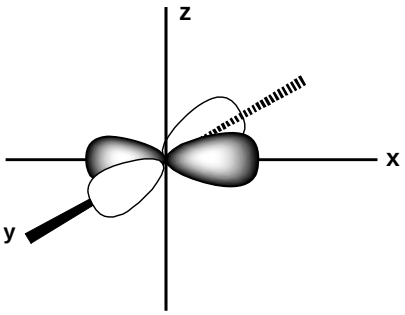
See slide 194 from Ch. 2 – the electrons to the right of the 4p do not shield the 4p

0.35 x 7 + 0.85 x 18 + 10 x 1 = 27.75 = σ

Zeff = Z-σ = 50-27.75 = 22.25

5. **(3 points)** We learned in class and from the text that we can only distinguish between areas of high-probability and low-probability for the electron density. We can be sure of the location of zero-probability features of the orbitals.
(a) **(2 point)** Sketch the 3d(x^2-y^2) orbital on the coordinate axes provided. Clearly indicate the phase of each lobe





b) (**1 point**) How many angular nodes does the 3d(x^2-y^2) have? *2*

6. a) **(1 point, no part marks)** Arrange the following in order of increasing ionization energy.

Na, K, Cl, P *Cl > P > Na >K*

b) **(1 point, no part marks)** Arrange the following in order of increasing (more negative) electron affinity.

P, Al, In, Cl *Cl > P > Al > In*

7. **(5 points)** Provide a detailed valence electronic configuration including the number of unpaired electrons for a phosphorus atom? Is this atom paramagnetic or diamagnetic? PCl_5 is a stable compound. Using your answer in part (a), provide a valence bond description (including hybridization) for the bonding in this compound.

$1s^2 2s^2 2p^6 3s^2 3p^3$ or $[Ne]3s^2 3p^3$

The three electrons in the 3p level are unpaired and thus the atom is paramagnetic

3points

See slide 153

Using unhybridized orbitals, P can only form 3 bonds to chlorine atoms. In order to make 5 bonds we will need 5 unpaired electrons. Promote one of the 3s electrons to the 3 d level. Hybridization of the 3s + 3x3p + 1x3d = dsp3 5 singly-occupied sp3d orbitals can now be used to make 5 P-Cl bonds

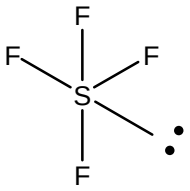
3p
3s

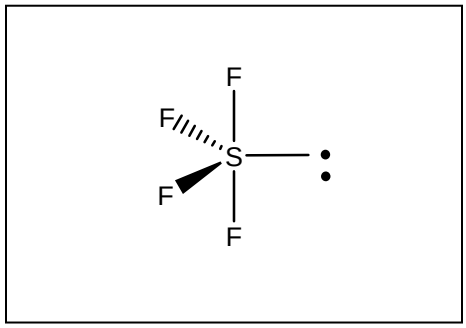
2points

8. (12 points, 1/2 point per blank; *no partial credit*) For the following molecules:
Draw the Lewis structure
Determine the VSEPR shape and geometry of the molecule
Draw the three-dimensional representation of the molecule in the box provided
Determine whether the molecule is polar or non-polar
Give the hybridization of the central atom
Indicate any ***non-zero formal charges*** on every element where they occur.

(a). SF_4 **3-D Drawing:**

LEWIS: *6 + 7x4 = 34 electrons*



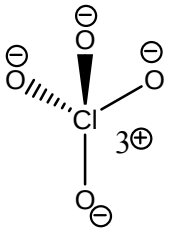


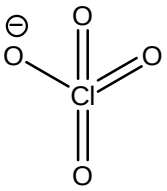
Geometry: _____tbp__ **Shape:** ___**seesaw**__ ____ _____

Polarity: _____yes____ _____ **Hybridization**:____dsp^3_____

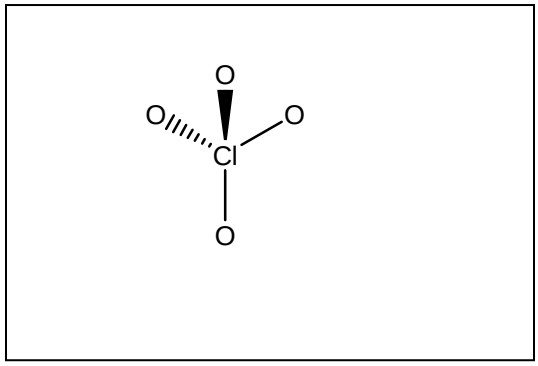
(b) **ClO_4^-** **3-D Drawing:**

LEWIS: 4x6+7+1 = 32 electrons





resonance!



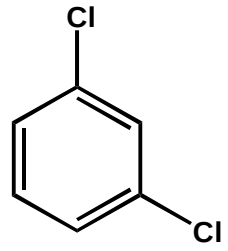
Geometry: _____Td_____ _____ **Shape:** _____**Td**_____

Polarity: _____no_____ **Hybridization:** ___sp^3_____

9. **(8 points, 1 points each; *no partial credit*)** For the following molecules or ions, indicate highest rotation axis and if there is a plane of reflection.
Example: BF_3 C_3, σh

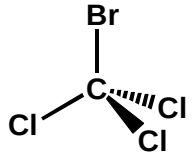
(a) N_3^- (a) C_∞, σh *and/or* σv

(b)



(b) C_2, σv

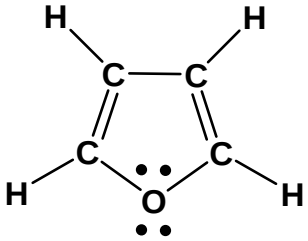
(c)



(c) C_3, σv

(d) NO_3^- (d) C_3, σh *and/or* σv

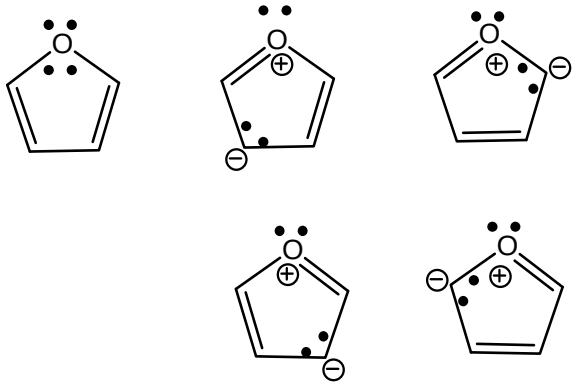
10. The following represents the Lewis structure and geometry of furan:



(**1 point**) What are the hybridizations of the carbon atoms in this depiction? sp^2

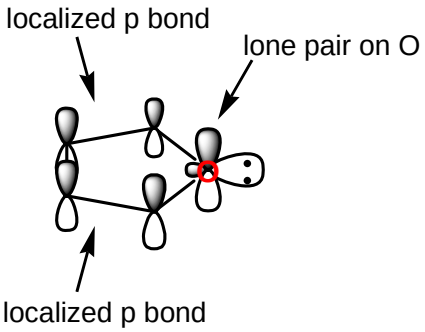
(**1 point**) Based on this drawing, how many σ-bonds and the π-bonds on the molecule? *9,2*

(2 points) Resonance structures for furan can be drawn by using the lone electron pairs on O for bonding with adjacent C. Draw a possible resonance structure with appropriate formal charges**.**



(2 points) Accounting for the additional resonance structures, what type of orbital must the lone electron pairs on oxygen be occupying? Explain.

If the lone pair is going to overlap with the p-bonding frame of the C atoms, it must be in a p orbital that lines up with these. This would give an sp^2 hybridized O. The remaining lone pair would be in an sp^2 hydbrid.



Useful equations, constants, and conversion factors:

$E = hc/\lambda$ $\qquad E = R_H\left(\frac{1}{n_l^2} - \frac{1}{n_h^2}\right)$ $\qquad E_{PIB} = \frac{n^2h^2}{8ma^2}$ $\qquad \psi_{PIB} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

$$[-(\frac{h^2}{8\pi^2 m})(\frac{d}{dx^2}^2 + \frac{d}{dy^2}^2 + \frac{d}{dz^2}^2) + V]\Psi = E\Psi \qquad \lambda = h/p$$

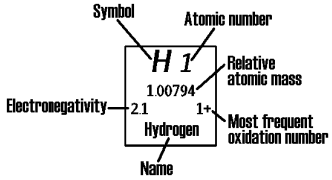
$\psi(r,\theta,\phi) = R(r)Y(\Theta, \Phi)$ The volume element is $r^2 \sin\Theta d\Theta d\Phi dr$

Angular wave functions: $Y(\Theta, \Phi) = (1/4\pi)^{1/2} y(\Theta, \Phi)$

orbital	$y(\Theta, \Phi)$
S	1
Pz	$3\cos\Theta$
px, py	$(2/3)^{1/2}\sin\Theta e^{\pm i\Phi}$
dz^2	$(5/4)^{1/2}(3\cos 2\Theta - 1)$
Dyz, dxz	$(15/4)^{1/2}\sin\Theta\cos\Theta e^{\pm i\Phi}$
$dx^2\text{-}y^2$,dxy	$(15/8)^{1/2}\sin 2\Theta\, e^{\pm 2i\Phi}$

h = Planck's constant = 6.626×10^{-34} J s
$R_H = 2.179 \times 10^{-18}$ J
1 m = 10^9 nm = 10^{12} pm
electron mass = 9.11×10^{-31} kg

c = speed of light = 2.998×10^8 m s^{-1}
Bohr radius (a_o) = 52.9 pm
1 J = 1 kg m^2 s^{-2}



	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIII	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	*H 1* 1.00794 2.1 1+ Hydrogen																	*He 2* 4.002602 - - Helium
2	**Li 3** 6.941 1.0 1+ Lithium	**Be 4** 9.012182 1.5 2+ Beryllium											**B 5** 10.811 2.0 3+ Boron	**C 6** 12.011 2.5 4+,4- Carbon	*N 7* 14.00674 3.0 3+,3- Nitrogen	*O 8* 15.9994 3.5 2- Oxygen	*F 9* 18.9984032 4.0 1- Fluorine	*Ne 10* 20.1797 - - Neon
3	**Na 11** 22.989768 0.9 1+ Sodium	**Mg 12** 24.3050 1.2 2+ Magnesium											**Al 13** 26.981539 1.5 3+ Aluminum	**Si 14** 28.0855 1.8 4+ Silicon	**P 15** 30.973762 2.1 5+ Phosphorus	**S 16** 32.066 1.8 4+ Sulfur	*Cl 17* 35.4527 3.0 1- Chlorine	*Ar 18* 39.948 - - Argon
4	**K 19** 39.0983 0.8 1+ Potassium	**Ca 20** 40.078 1.0 2+ Calcium	**Sc 21** 44.955910 1.3 3+ Scandium	**Ti 22** 47.88 1.5 4+ Titanium	**V 23** 50.9415 1.6 5+ Vanadium	**Cr 24** 51.9961 1.6 3+ Chromium	**Mn 25** 54.93805 1.5 2+ Manganese	**Fe 26** 55.847 1.8 3+ Iron	**Co 27** 58.9332 1.8 2+ Cobalt	**Ni 28** 58.6934 1.8 2+ Nickel	**Cu 29** 63.546 1.9 2+ Copper	**Zn 30** 65.39 1.6 2+ Zinc	***Ga 31*** 69.723 1.6 3+ Gallium	**Ge 32** 72.61 1.6 4+ Germanium	**As 33** 74.92159 2.0 3+,3- Arsenic	**Se 34** 78.96 2.4 4+ Selenium	***Br 35*** 79.904 2.8 1- Bromine	*Kr 36* 83.80 - - Krypton
5	**Rb 37** 85.4678 0.8 1+ Rubidium	**Sr 38** 87.62 1.0 2+ Strontium	**Y 39** 88.90585 1.3 3+ Yttrium	**Zr 40** 91.224 1.4 4+ Zirconium	**Nb 41** 92.90638 1.6 5+ Niobium	**Mo 42** 95.94 1.8 6+ Molybdenum	Tc 43 98.9063 1.9 7+ Technetium	**Ru 44** 101.57 2.2 3+,4+ Ruthenium	**Rh 45** 102.9055 2.2 3+ Rhodium	**Pd 46** 106.42 2.2 2+ Palladium	**Ag 47** 107.8682 1.9 1+ Silver	**Cd 48** 112.411 1.7 2+ Cadmium	**In 49** 114.82 1.7 3+ Indium	**Sn 50** 118.71 1.8 4+ Tin	**Sb 51** 121.757 1.9 3+,3- Antimony	**Te 52** 127.60 2.1 4+ Tellurium	**I 53** 126.90447 2.5 1- Iodine	*Xe 54* 131.29 - - Xenon
6	***Cs 55*** 132.90543 0.7 1+ Cesium	**Ba 56** 137.327 0.9 2+ Barium	**La 57** 138.9055 1.1 3+ Lanthanum	**Hf 72** 178.49 1.3 4+ Hafnium	**Ta 73** 180.9479 1.5 5+ Tantalum	**W 74** 183.85 1.7 6+ Tungsten	**Re 75** 186.207 1.9 7+ Rhenium	**Os 76** 190.2 2.2 4+ Osmium	**Ir 77** 192.22 2.2 4+ Iridium	**Pt 78** 195.08 2.2 4+ Platinum	**Au 79** 196.96654 2.4 3+ Gold	***Hg 80*** 200.59 1.9 2+ Mercury	**Tl 81** 204.3833 1.8 1+ Thallium	**Pb 82** 207.2 1.8 2+ Lead	**Bi 83** 208.98037 1.9 3+ Bismuth	**Po 84** 208.9824 2.0 2+ Polonium	**At 85** 209.9871 2.2 1- Astatine	*Rn 86* 222.0176 - - Radon
7	***Fr 87*** 223.0197 0.7 1+ Francium	**Ra 88** 226.0254 0.9 2+ Radium	**Ac 89** 227.0278 1.1 3+ Actinium	Rf 104 261.11 - - Rutherfordium	Db 105 262.11 - - Dubnium	Sg 106 263.12 - - Seaborgium	Bh 107 262.12 - - Bohrium	Hs 108 264 - - Hassium	Mt 109 266.1378 - - Meitnerium	Uun 110 269 - - Ununnilium	Uuu 111 272 - - Unununium	Uu 112 277 - - Ununbium		Uuq 114 289 - - Ununquadium		Uuh 116 289 - - Ununhexium		Uuo 118 293 - - Ununoctium

6	**Ce 58** 140.115 1.1 3+ Cerium	**Pr 59** 140.90765 1.1 3+ Praseodymium	**Nd 60** 144.24 1.1 3+ Neodymium	Pm 61 144.9127 1.1 3+ Promethium	**Sm 62** 150.36 1.2 3+ Samarium	**Eu 63** 151.965 1.2 3+ Europium	**Gd 64** 157.25 1.2 3+ Gadolinium	**Tb 65** 168.92534 1.2 3+ Terbium	**Dy 66** 162.50 1.2 3+ Dysposium	**Ho 67** 164.93032 1.2 3+ Holmium	**Er 68** 167.26 1.2 3+ Erbium	**Tm 69** 168.93421 1.2 3+ Thulium	**Yb 70** 173.04 1.1 3+ Ytterbium	**Lu 71** 174.967 1.2 3+ Lutetium
7	**Th 90** 232.0381 1.3 4+ Thorium	**Pa 91** 231.03588 1.5 5+ Protactinium	**U 92** 238.0289 1.4 6+ Uranium	Np 93 237.082 1.3 5+ Neptunium	Pu 94 244.0642 1.3 4+ Plutonium	Am 95 243.0614 1.3 3+ Americium	Cm 96 247 1.3 3+ Curium	Bk 97 247.0703 1.3 3+ Berkelium	Cf 98 251.0796 1.3 3+ Californium	Es 99 252.03 1.3 - Einsteinium	Fm 100 257.0951 1.3 - Fermium	Md 101 258.01 1.3 - Mendelevium	No 102 259.1009 1.3 - Nobelium	Lr 103 260.1053 - - Lawrencium

Under normal conditions, bold symbols correspond to solid state, bold italic correspond to liquid state, italic correspond to gaseous state and normal correspond to synthetic elements.