

Please follow the instructions for each section of the exam. Show your work on all mathematical problems. Provide answers with the correct units and significant figures. Be concise in your answers to discussion questions.

**Part 0: Warmup. 4 points each**

1. Which of the following electronic transitions in a hydrogen atom results in the emission of light of the highest frequency?

- a.  $n = 4$  to  $n = 3$
- b.  $n = 2$  to  $n = 1$
- c.  $n = 6$  to  $n = 1$
- d.  $n = 3$  to  $n = 2$

Answer   c  

2. Which of the following has the largest diameter?

- a. argon atom
- b. potassium ion
- c. calcium ion
- d. chloride ion

Answer   d  

**Part I: Complete all of problems 3-6**

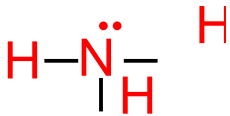
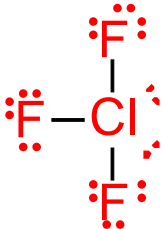

3. Define the following using a maximum of two sentences for each definition. (12 points)

- a. resonance: Resonance is invoked when two or more reasonable Lewis Structures can be drawn for a single species. The real structure is a hybrid on the different contributing structures.
- b. radial node: Region in space a constant distance from the nucleus where there  $\psi^2$  (probability of finding an electron) is zero.
- c. wavefunction: Mathematical expression that describes a solution to the Schrodinger equation and reflects an orbital for an electron in an atom (typically hydrogen).

4. Write the ground state electron configurations for the following species. You may choose to use noble gas notation if you wish. (12 points)

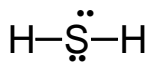
a. Iodine	$[\text{Kr}]5s^24d^{10}5p^5$
b. sulfide ion	$[\text{Ar}]$
c. chromium	$[\text{Ar}]4s^13d^5$
d. iron (II) ion	$[\text{Ar}]3d^6$

5. Complete the table for **two (2)** of the species below: (12 points)

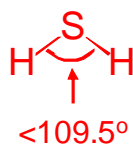
Species	Lewis Structure (indicate resonance if necessary)	Electron Pair Geometry	Molecular Geometry	Polar Molecule? (yes/no)
NH <sub>3</sub>		tetrahedral	trigonal pyramidal	yes
ClF <sub>3</sub>		trigonal bipyramidal	T-shaped	yes
SO <sub>2</sub>		trigonal planar	bent	yes

6. Below are the Lewis structures for two compounds. For each compound, name the molecular geometry and provide a three dimensional sketch of the compound. Indicate approximate bond angles (12 points)

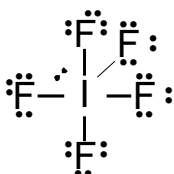
a. H<sub>2</sub>S



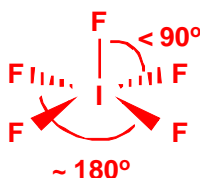
Bent molecular geometry



b. IF<sub>5</sub>

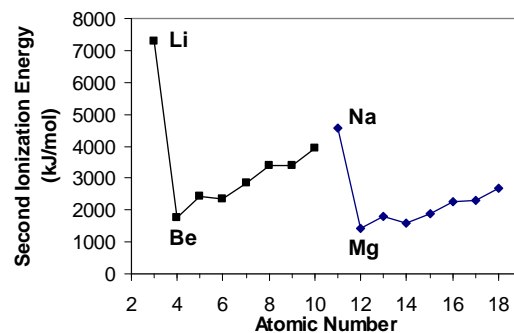


Square pyramidal geometry



**Part II. Answer three (3) of problems 7-10. Clearly mark the problem you do not want graded. 15 points each.**

7. Consider the general trends in second ionization energy, as shown in the figure to the right. The second ionization energy is for the reaction:



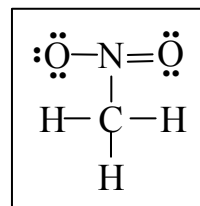
- a. Why are the second ionization energies of the group two atoms (Li-Ne) larger than those of the group three atoms (Na-Ar)?

In general, period two elements have a larger effective nuclear charge than the elements below them in period three. This is due, in part, to the fact that there are fewer electrons available to shield the charge of the nucleus. With this larger  $Z^*$ , it is more difficult to remove an electron (or two electrons as is this case) from the elements in the second row than for those in the third.

- b. Why is there a large decrease from Li to Be and then a general increase as you move across the group to Ne?

For the jump from Be to Li, the second ionization energy requires the formation of  $Li^{2+}$  from  $Li^+$ . Since both  $Li^+$  has a noble gas configurations, there is a large price to pay in energy.

8. Organic compounds containing nitro groups (-NO<sub>2</sub>) often possess very explosive characteristics. Nitromethane (CH<sub>3</sub>NO<sub>2</sub>) is the simplest of these nitrated organic compounds. It undergoes combustion by the following reaction



The Lewis structure of nitromethane is shown at the right. Using the table of bond dissociation energies on the last page of the exam, determine the  $\Delta H^\circ$  for this reaction.

In order to rearrange the atoms in the reactants to form products, we need to break and make the following bonds:

**Bonds Broken:**

<b>Bond</b>	N-O	N=O	C-N	C-H	O=O	
<b>Quantity</b>	2	2	2	2x3 = 6	1	<b>Total</b>
<b>Energy (kJ)</b>	2(201)	2(852)	2(305)	6(413)	498	<b>5692</b>

**Bonds Formed:**

<b>Bond</b>	C=O	H-O	N≡N	
<b>Quantity</b>	2x2 = 4	2x2 = 4	1	<b>Total</b>
<b>Energy (kJ)</b>	4(732)	4(463)	945	<b>5725</b>

$$\Delta H^\circ = (\text{Total for bonds broken}) - (\text{Total for bonds formed}) = 5692 - 5725 = -33 \text{ kJ}$$

**Now with the correctly balanced reaction!**



**Bonds Broken:**

<b>Bond</b>	N-O	N=O	C-N	C-H	O=O	
<b>Quantity</b>	4	4	4	4x3 = 12	3	<b>Total</b>
<b>Energy (kJ)</b>	4(201)	4(852)	4(305)	12(413)	3(498)	<b>11882</b>

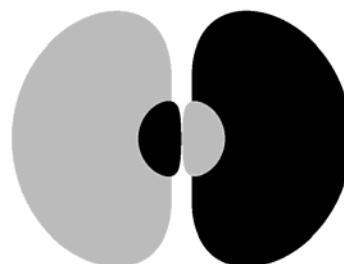
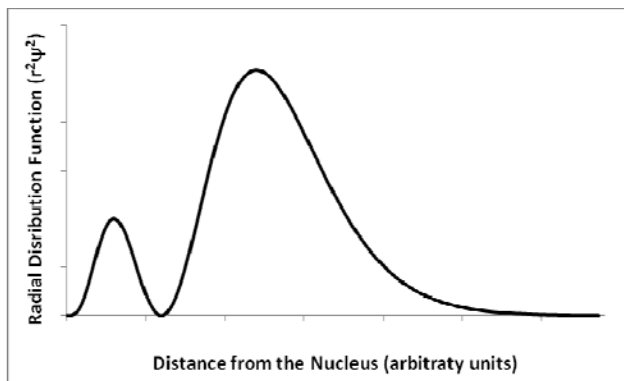
**Bonds Formed:**

<b>Bond</b>	C=O	H-O	N≡N	
<b>Quantity</b>	4x2 = 8	6x2 = 12	2	<b>Total</b>
<b>Energy (kJ)</b>	8(732)	12(463)	2(945)	<b>13302</b>

$$\Delta H^\circ = (\text{Total for bonds broken}) - (\text{Total for bonds formed}) = 11882 - 13302 = -1420 \text{ kJ}$$



10. Consider the following diagrams of the same orbital. Which orbital do the pictures represent? Provide the values for  $n$ ,  $\ell$ , and  $m_\ell$  for the orbital and *justify your reasoning*.



To assign values for  $n$  and  $\ell$ , we need to look for nodes in the orbitals. From the probability plot on the right, it appears that there are one angular node in this orbital. For this to be true, the value of  $\ell$  must be 1, resulting in a **p** orbital. From the plots above, we observe only one radial node in the orbital, as evidenced by the one location outside the nucleus where the Distribution Function is zero (above left) and the one circular interface between the grey and black phases in the Probability Density plot (above right). Therefore  $n - \ell - 1$  must equal 1. If  $\ell = 1$ , then the value of  $n$  must be **3**. With  $n = 3$ , and  $\ell = 1$ , we must have a **3p** orbital. The third quantum number,  $m_\ell$  depends on the value of  $\ell$  ( $m_\ell$  ranges from  $-\ell$  through zero to  $+\ell$ ). Since  $\ell=1$  for this orbital, there are three possible value of  $m_\ell$  (1-, 0, +1). Any of the three values will be acceptable So,

$$\begin{aligned} n &= 3 \\ \ell &= 1 \\ m_\ell &= -1, 0, +1 \end{aligned}$$

### Possibly Useful Information

$h = 6.63 \times 10^{-34} \text{ Js}$	$c = 3.00 \times 10^8 \text{ m/s}$	$R_H = 2.179 \times 10^{-18} \text{ J/atom}$
$E = h\nu$	$\nu\lambda = c$	$\Delta E \cdot \Delta(mv) > h$
$H\psi = E\psi$	$E = -\frac{R_H}{n^2}$	$\Delta E = -R_H \left( \frac{1}{n_{\text{final}}^2} - \frac{1}{n_{\text{initial}}^2} \right)$

**TABLE 10.3 Some Average Bond Energies<sup>a</sup>**

Bond	Bond Energy, kJ/mol	Bond	Bond Energy, kJ/mol	Bond	Bond Energy, kJ/mol
H—H	436	C—C	347	N—N	163
H—C	414	C=C	611	N=N	418
H—N	389	C≡C	837	N≡N	946
H—O	464	C—N	305	N—O	222
H—S	368	C=N	615	N=O	590
H—F	565	C≡N	891	O—O	142
H—Cl	431	C—O	360	O=O	498
H—Br	364	C=O	736 <sup>b</sup>	F—F	159
H—I	297	C—Cl	339	Cl—Cl	243
				Br—Br	193
				I—I	151

1																	18
1A																	8A
1 H 1.00794	2 2A											13 3A	14 4A	15 5A	16 6A	17 7A	2 He 4.00260
3 Li 6.941	4 Be 9.01218											5 B 10.811	6 C 12.011	7 N 14.0067	8 O 15.9994	9 F 18.9984	10 Ne 20.1797
11 Na 22.9898	12 Mg 24.3050	3B	4B	5B	6B	7B	8B		10	11 1B	12 2B	13 Al 26.9815	14 Si 28.0855	15 P 30.9738	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.9559	22 Ti 47.88	23 V 50.9415	24 Cr 51.9961	25 Mn 54.9381	26 Fe 55.847	27 Co 58.9332	28 Ni 58.693	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.9216	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.9059	40 Zr 91.224	41 Nb 92.9064	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.906	46 Pd 106.42	47 Ag 107.868	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.757	52 Te 127.60	53 I 126.904	54 Xe 131.29
55 Cs 132.905	56 Ba 137.327	57 *La 138.906	72 Hf 178.49	73 Ta 180.948	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.967	80 Hg 200.59	81 Tl 204.383	82 Pb 207.2	83 Bi 208.980	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.025	89 †Ac 227.028	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (271)	111 Rg (272)							

*Lanthanide series	58 Ce 140.115	59 Pr 140.908	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.965	64 Gd 157.25	65 Tb 158.925	66 Dy 162.50	67 Ho 164.930	68 Er 167.26	69 Tm 168.934	70 Yb 173.04	71 Lu 174.967
†Actinide series	90 Th 232.038	91 Pa 231.036	92 U 238.029	93 Np 237.048	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

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