

HW Set 1

- 1) Tetradentate ligand: A ligand that coordinates a metal at four sites (atoms).
- 2) Blue solution absorbs between 580-650nm.

Chapter 2

1)

$$R = K_{2s} \left(2 - \frac{Zr}{a_0} \right) e^{-\frac{Zr}{a_0}} = 0 \rightarrow \text{Node}$$

$$2 - \frac{Zr}{a_0} = 0 ; \quad r = \frac{2a_0}{Z} ; \quad Z = 1$$

$$r = 2a_0$$

$$r = 2(52.93 \text{ pm}) = 105.86 \text{ pm}$$

2) a. Shape: l

b. Energy: n → H type atom

n + l → for polyelectronic atoms

c. Orientation: m_l

d. Size of orbitals: n

3) How many orbitals for n=4?

n = 4

l = 0, 1, 2, 3 4 types of orbitals

$$4s, \underbrace{4p}_{p_x, p_y, p_z}, \underbrace{4d}_{5 \text{ orbitals}}, \underbrace{4f}_{7 \text{ orbitals}} \Rightarrow 16 \text{ orbitals}$$

4) radial nodes: $n - l - 1$
angular nodes: l

nodes	3s	4p	3d	5f
radial	2	2	0	1
angular	0	1	2	3

5) $n = 5$

$l = 0, 1, 2, 3, 4$ $5s^2 5p^6 5d^{10} 5f^{14} 5g^{18} = 50$

$m_l = -4, -3, -2, -1, 0, 1, 2, 3, 4$

$m_s = \pm \frac{1}{2}$

$n = 5, l = 4, m_l = 4, m_s = \pm \frac{1}{2}$ possible quantum #

6) p^3



$S = 1.5$

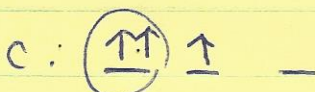
$2S + 1 = 4$

maximum multiplicity

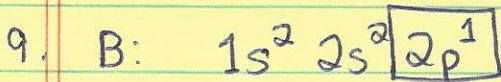
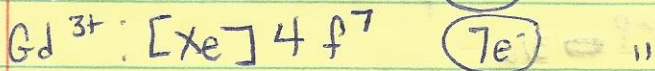
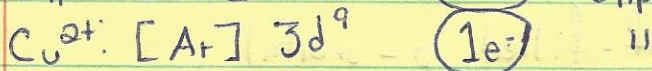
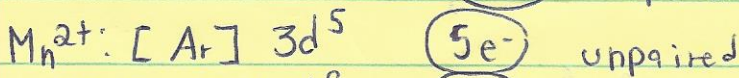
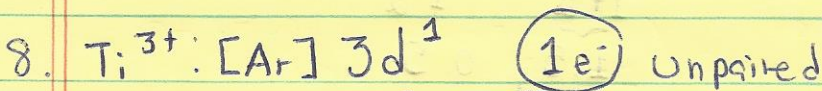
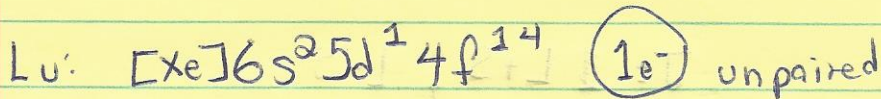
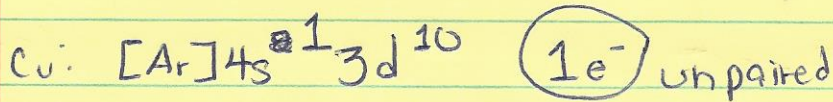
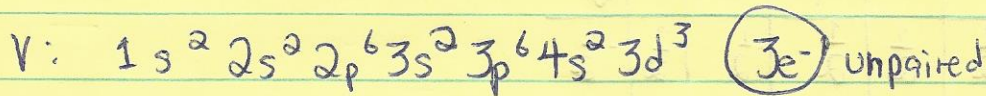
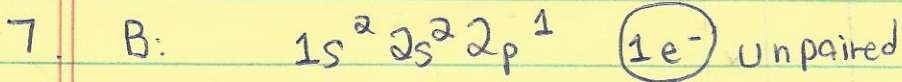
Ground state because maximum multiplicity and least exchange energy and coulombic repulsion



coulombic repulsion



impossible



m_l : $\begin{matrix} \uparrow \\ +1 & 0 & -1 \end{matrix}$

$L = 1 \rightarrow P$ state

$M = 2(\frac{1}{2}) + 1 = 2$ Term symbol 2P for ground state
but not complete

$x = 1$

$l = 1$

$N_l = 2(2(1) + 1) = 6$

of microstates = $\frac{6!}{1!5!} = 6$

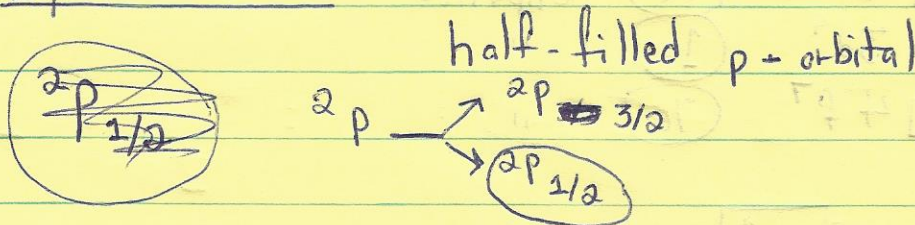
M	L	1	0	-1	1	0	-1
		↑			↓		
m_l		0	↑			↓	
		-1		↑			↓
M	S	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$

	M_s	$\frac{1}{2}$	$-\frac{1}{2}$
M_l	1	(X)	(X)
	0	(X)	(X)
	-1	(X)	(X)

$J = L + S, L - S$

$1 + \frac{1}{2}, 1 - \frac{1}{2}$

$\frac{3}{2}, \frac{1}{2}$



$N: 1s^2 2s^2 2p^3$

m_l	↑	↑	↑
	+1	0	-1

$L = 0 \rightarrow s$ state

$M = 2(\frac{3}{2}) + 1 = 4$ Term symbol 4S for ground state but not complete

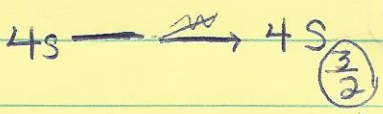
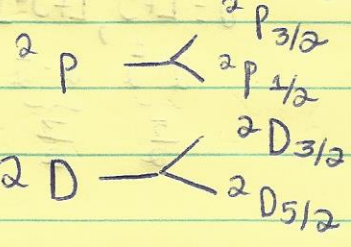
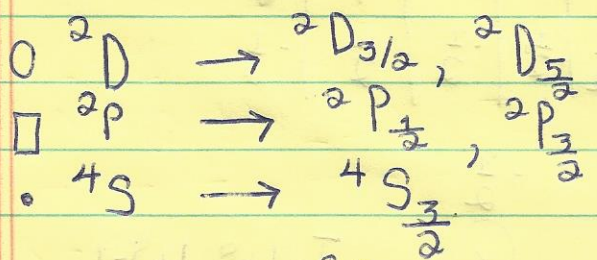
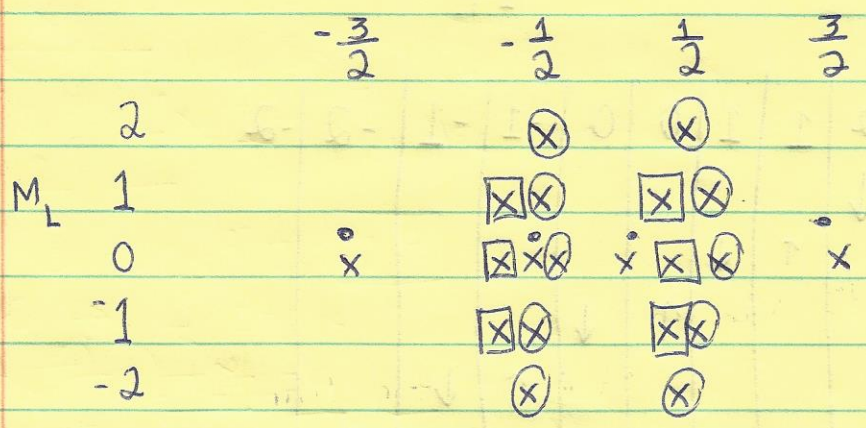
$\chi = 3$

$l = 1$

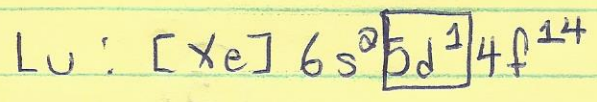
$N_l = 2(2(1) + 1) = 6$

~~oooo~~
 # of microstates = $\frac{6!}{3!(3!)} = 20$

M_L	0	0	0	0	0	0	2	2	1	1	1	1	-1	-1	-1	-1	-2	-2	0	0	
m_s	↑	↑	↑	↓	↓	↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↓	
	↑	↑	↓	↑	↓	↓	↑	↓			↑↓	↑↓	↑↓	↑↓			↑	↓	↓	↑	
	↑	↓	↑	↑	↑	↓			↑	↓			↑	↓	↑↓	↑↓	↑↓	↑↓	↑↓	↓	↓
M_S	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$



half-filled orbital



m_l \uparrow
 +2 +1 0 -1 -2

$L = 2 \rightarrow D$ state

$S = \frac{1}{2}$ $M = 2(\frac{1}{2}) + 1 = 2$

²D would be the ground state

$x = 1$

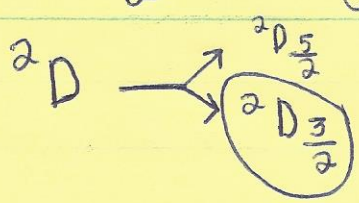
$l = 2$

$N_l = 2(2(2)+1) = 10 \rightarrow \frac{10!}{1!9!} = 10$ microstates

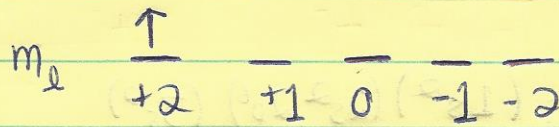
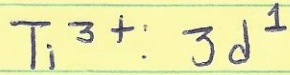
M_L	2	2	1	1	0	0	-1	-1	-2	-2
m_l	\uparrow	\downarrow	\uparrow	\downarrow	\uparrow	\downarrow	\uparrow	\downarrow	\uparrow	\downarrow
M_S	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$

	$\frac{1}{2}$	$-\frac{1}{2}$
+2	(X)	(X)
+1	(X)	(X)
0	(X)	(X)
-1	(X)	(X)
-2	(X)	(X)

$J = L+S, L+S-1$
 $2+\frac{1}{2}, 2-\frac{1}{2}$
 $\frac{5}{2}, \frac{3}{2}$



7



L = 2 → D state

S = +1/2 M = 2(1/2) + 1 = 2 → ²D

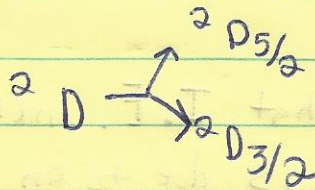
x = 1

l = 2

N_e = 2(2(2)+1) = 10

→ 10! / 1!9! = 10 microstates

So no different than the Lu example.



10. a. 3p e⁻ in P ⇒ (1s²)(2s², 2p⁶)(3s², 3p³)

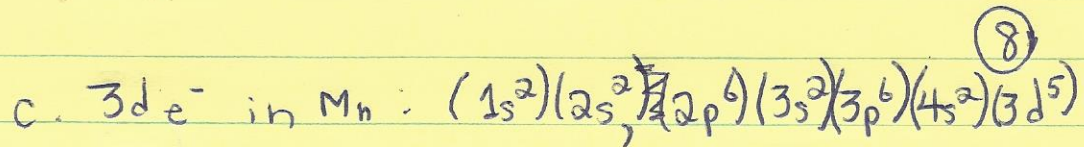
S = 0.35(4) + 0.85(8) + 1(2) = 10.2

Z* = Z - S = 15 - 10.2 = 4.8

b. 4s e⁻ in Co: (1s²)(2s², 2p⁶)(3s², 3p⁶)(3d⁷)(4s²)

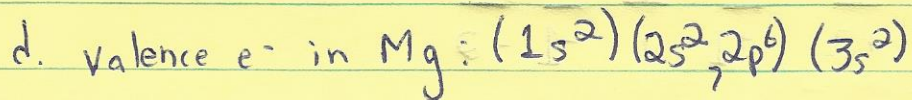
S = (1 × 0.35) + (15 × 0.85) + 10(1.00) = 23.10

Z* = 27 - 23.10 = 3.90



$$S = 0.35(4) + 1.00(18) = 19.40$$

$$Z^* = 25 - 19.40 = 5.60$$



$$S = 0.35 + 0.85(8) + 2.00 = 9.15$$

$$Z^* = 12 - 9.15 = 2.85$$

11. a. Li

b. F

c. Cu

d. Pt

12. A general trend is that I.E. increases as n increases. This is due to an increase in effective nuclear charge felt by the remaining e^- after an electron is removed because of greater electrostatic attraction between the positive nucleus and the electrons.

A significant jump in I.E. is noticed between the values of $n=3$ + $n=4$. The e^- up to $n=3$ are those that pertain to orbitals of primary quantum # 3, which means they are higher in energy

and it is easier for e^- to be removed from them. The remaining e^- of the plot are removed from orbitals pertaining to primary quantum #2. It is even harder to remove e^- from orbitals in this shell.

- 13) a. Li
- b. F
- c. Cl
- d. S

Chapter 18

2) Many separation methods (i.e. ion-exchange chromatography) rely on differences in charge/size ratios. Because of the lanthanide contraction in addition to the relativistic effect, Zr^{4+} + Hf^{4+} are virtually the same size. Since they have the same charge, separation methods that rely on charge/size differences will not be able to distinguish between them.

4) a. Electron affinities increase from left to right as $\uparrow Z^*$.

But take the periodic anomalies into consideration.

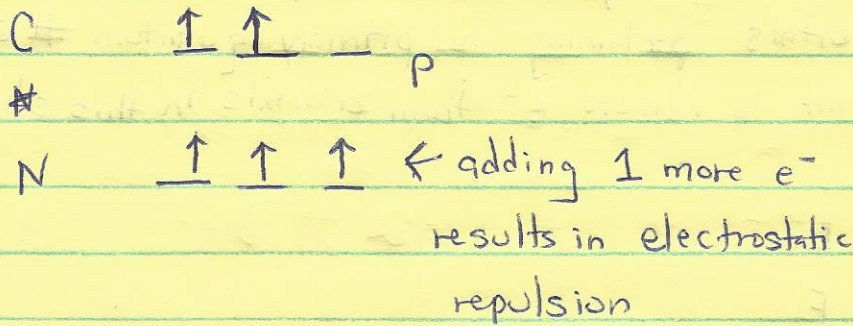
b. Ionization energies increase as the value of n increases.

c. Atomic radii increase as $\uparrow n$ while $\uparrow Z^*$ slowly.

d. Atomic radii decreases from left to right because $\Delta n = 0$ and $\uparrow Z^*$ increases.

e. skip → We did not discuss this fully.

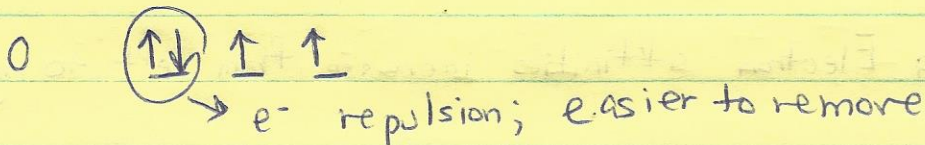
8) C-N: N has a lower EA because



Na-Mg: Mg lower EA because extra e^- must enter a 2p orbital → higher in energy

Cu-Zn: Zn lower EA because extra e^- must enter a 4p orbital, which ~~feels a~~ Also ~~would disrupt its s~~ for Cu, Cu would obtain \uparrow filled d-orbitals → very stable

9) N-O: Oxygen has a lower I.E.

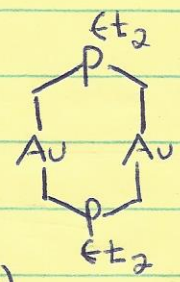


Be-B : B has lower I.E. because outer e⁻ is in a 2p orbital → higher energy orbital.
For Be, outer e⁻ in s orbital.

Mg-Al: Al has lower I.E. b/c its outer e⁻ is in a 3p orbital where as for Mg it is in a 3s.

P-S: Same as for N-O

Zn-Ga: Ga has lower IE b/c its outer e⁻ is in a 4p orbital where ~~for~~ for Zn it is in a 3d.

18) In the molecule  gold engages in a mostly (if not entirely) covalent bond because

$\Delta\chi$ between Au (~~2.54~~^{2.54}) + C (2.55) is virtually 0. Because of the covalency of the bond, Au would not be expected to have a true formal oxidation state of +1.