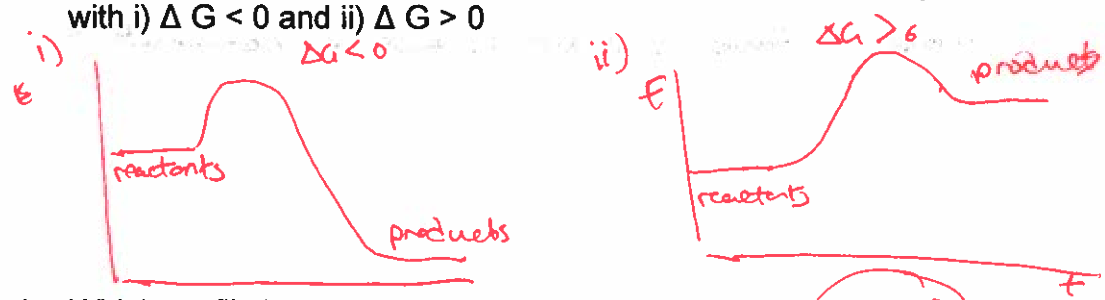
PLTL Worksheet #1:
Thermochemistry, Periodic Trends, Electronic Structure, Orbitals, Bonding

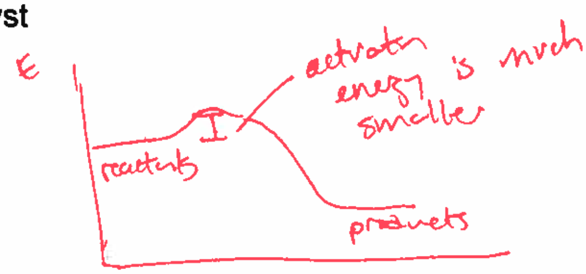
1. *Thermochemistry Review*

   a. Use the space below to draw reaction energy profiles for a system with i) Δ G < 0 and ii) Δ G > 0



   b. Which profile indicates a spontaneous reaction? ΔG<0

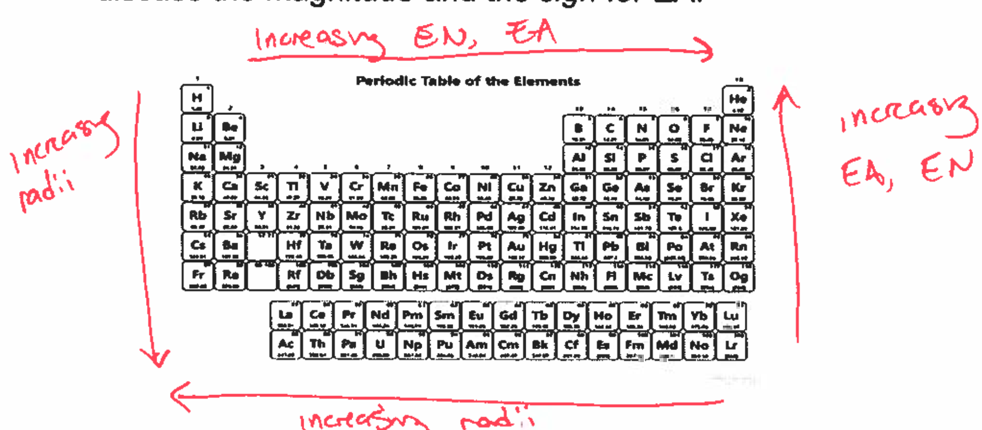
   c. Draw a reaction energy profile for a reaction under the effect of a catalyst



2. *Periodic Trends*

   a. Draw arrows on the periodic table to illustrate the following trends: i) Atomic Radii ii) Electron Affinity iii) Electronegativity.

   b. Briefly explain the reason these trends are observed. Be sure to discuss the magnitude and the *sign* for EA.



b) i) increasing quantum #, increased distance of valence e⁻. Decreases across due to ↑ prot resulting in greater nuclear pull

iii) increases across b/c stronger attraction from nucleus
decreases going down b/c greater distance between nucleus & valence shell

→ see back for EA

(ii) Note:

EA is the energy change of when an atom gains an electron.

or

energy needed to remove e⁻ from (-)ve anion

- High electron affinity = becoming more stable when e⁻ is added

= negative energy

→ reason for trends is similar to that of electronegativity

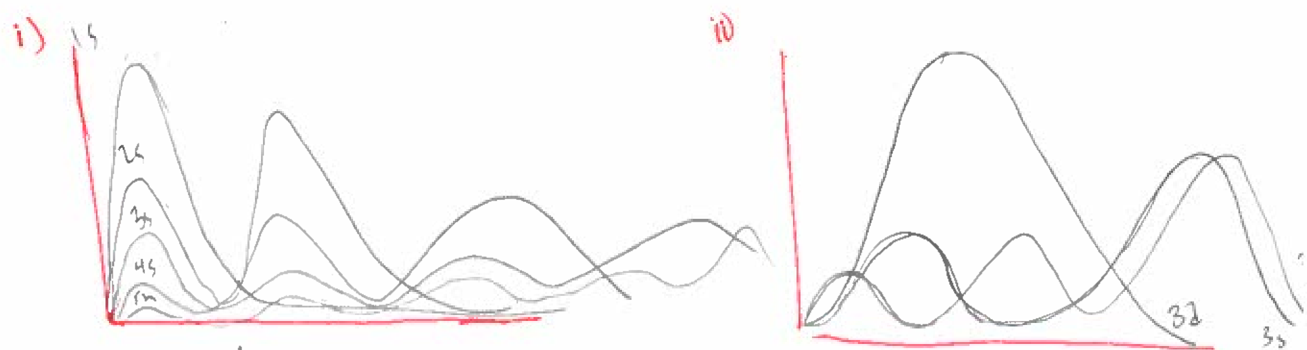
c. For each of the following, indicate which element has the *greater* first ionization energy, and explain why

Be vs B — Be has full shell

Kr vs Xe — larger atom more shielded from nuclear attraction

Na vs K

3. *Orbitals and Electronic Configuration*
   a. Using the space below, draw the radial probability density plots for i) 1s, 2s, 3s, 4s, 5s ii) 3s, 3p, 3d



* note # of nodes

b. State the quantum numbers for the following orbitals:

i. 3s n = 3 , l = 0

ii. 3p n = 3 , l = 1

iii. 3d n = 3 , l = 2

c. Give the electron configuration for iron in the following species, using core notation

i. $Fe^0(g)$ [Ar] $4s^2 3d^6$

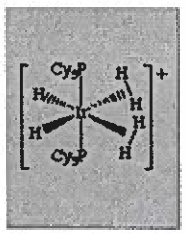
ii. Fe^{II} as in $Fe(H_2O)_6^{2+}$ [Ar] $3d^6$

iii. $Fe^0(CO)_5$ [Ar] $3d^8$

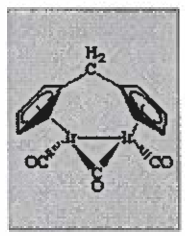
iv. Fe^{III} as in $FeCl_4^-$ [Ar] $3d^5$

4. *Electron Counting (EXTRA PRACTICE)*

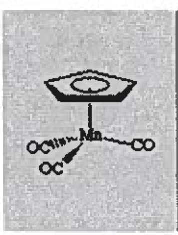
Using the neutral counting method, determine the total valence electron count for the following molecules:



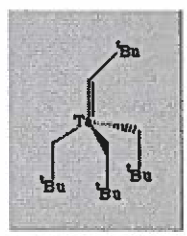
Ir → 9e⁻
2 H → 2e⁻
2 H_2 → 4e⁻
2 PCy_3 → 4e⁻
1 (+)ve charge → minus 1e⁻
(18e⁻)



• Ir → 9e⁻
Cp → 5e⁻
CO (terminal) → 2e⁻
CO (Bridging) → 1e⁻
Ir – Ir bond → 1e⁻
(18e⁻)

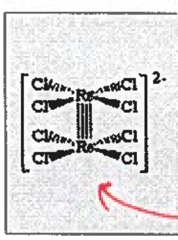


Mn → 7e⁻
Cp⁻ → 5e⁻
3 CO → 6e⁻
(18e⁻)

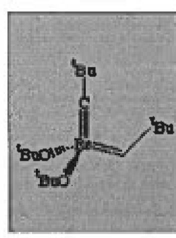


Ta → 5e⁻
3 ᵗBuCH₂ → 3e⁻
ᵗBuCH → 2e⁻
(10e⁻)

* M–M bonds are simply e⁻ pairs

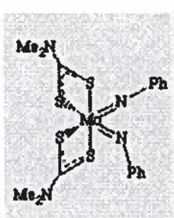


Re → 7e⁻
4 Cl → 4e⁻
4 Re–Re bonds → 4e⁻
1 (−)ve charge → 1e⁻
(16e⁻) for one Re

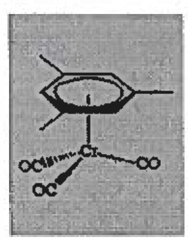


~~Ta → 5e⁻~~
~~3 ᵗBuCH₂ → 3e⁻~~
~~ᵗBuCH → 2e⁻~~
~~(10e⁻)~~

Re → 7e⁻
RHC → 2e⁻
R–C → 3e⁻
2 R–O → 6e⁻
(18e⁻)

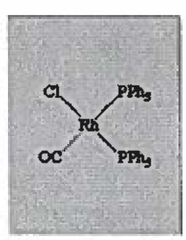


Mo → 6e⁻
linear PhN → 4e⁻
bent PhN → 2e⁻
2 dtc ligands → 6e⁻
(18e⁻)



Cr → 6e⁻
arene (neutral) → 6e⁻
3 CO → 6e⁻
(18e⁻)

Co → 9e⁻
2 Cp → 10e⁻
(19e⁻)



Rh → 9e⁻
Cl → 1e⁻
CO → 2e⁻
2 PPh_3 → 4e⁻
(16e⁻)

CHEM 362 – Fall 2019
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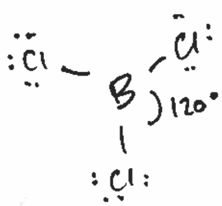
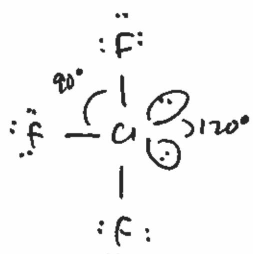
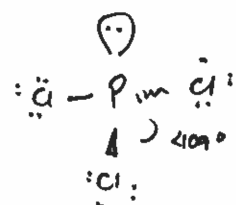
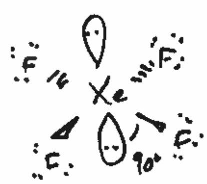
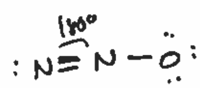
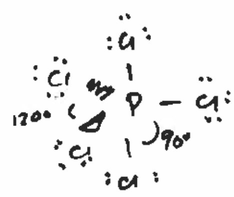
5. *Structure and Bonding*
   a. Give the Lewis structures and by VSEPR predict the shapes of the species below. Draw the geometrical structures and give all angles.

BCl_3	ClF_3	PCl_3
		
XeF_4	N_2O	PCl_5
		

   b. Predict the hybridization of orbitals required for the central atom to make localized valence bonds in each of the above.

BCl_3 sp^2　　　XeF_4 sp^3d^2

ClF_3 sp^3d　　　N_2O sp

PCl_3 sp^3　　　PCl_5 sp^3d