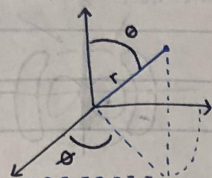


MIDTERM: CHEM 121

Chapter 5:



r = length of vector
 θ = angle between vector and z-axis
 ϕ = angle between the projected vector on the xy plane and x-axis

QUANTUM NUMBERS: the set of numerical values in a wave function that gives valid solutions to the Schrodinger equation. (n, l, m_l)

① Principal quantum number (n). n can be any positive integer, $n = 1, 2, 3$

- defines the shell
- determines the energy of an orbital

② Orbital Angular momentum quantum number (l). l can equal to anything $n-1$

- defines the subshell
- determines shape of orbital

$l = 0$: s	$l = 3$: f
$l = 1$: p	$l = 4$: g
$l = 2$: d	$l = 5$: h

③ Magnetic quantum number (m_l). $m_l = -l, \dots, +l$

- defines a particular orbital

Ex. In orbital with $n = 3$ and $m_l = -1$, what are the allowed values of l ?

$n = 3 \rightarrow l$ can be 0, 1, or 2

$m_l = 2, -1, 0, 1, 2 \rightarrow l$ must be 1 or 2

$\rightarrow l = \#$ of angular nodes

In the s-orbital, $l = 0 \therefore$ no angular nodes

p-orbital, $l = 1 \therefore$ one angular node

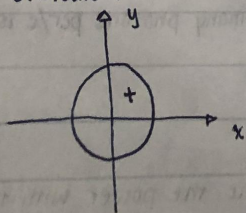
Total nodes = # of radial nodes + # angular nodes

$(n-1)$

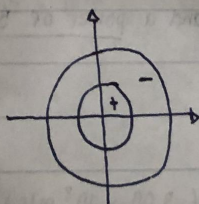
(l)

Cross-section diagrams

s-orbitals:



1s



2s

$(n-1) = 1$ radial node

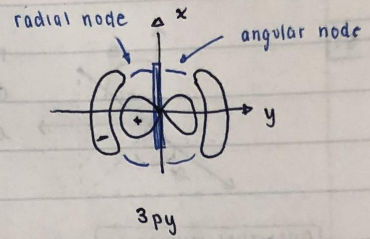
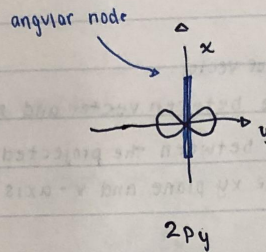
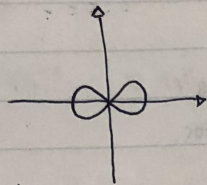
p - orbitals :

Generic shape :

! has one angular node

$$l = 1 \text{ so } m_l = -1, 0, 1$$

(p_x, p_y, p_z)



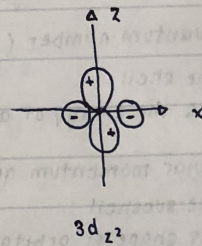
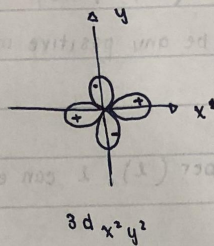
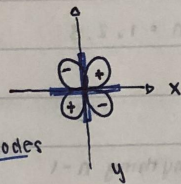
d - orbitals :

Generic shape :

! has two angular nodes

$$l = 2 \text{ so } m_l = -2, -1, 0, 1, 2$$

($d_{xy}, d_{xz}, d_{yz}, d_{x^2}, d_{x^2-y^2}$)



Chapter 6:

Definitions

Monochromatic : light that consists of only waves with the same wavelength

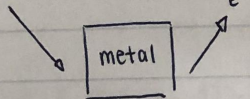
Coherent : when multiple light waves have the same wavelength and are produced at the same time

Incoherent : when multiple light waves have different wavelengths produced at random times

Linearly polarized light : have waves that have their electric field components vibrating at the same plane

What is the photoelectric effect?

light ($h\nu$)



=> when light ($h\nu$) is shone on a piece of metal, electrons can be ejected from the surface of the metal if the energy is large enough.

$E = h\nu$ is the Planck Relation; this equation tells us that the energy of a photon is directly proportional to the frequency.

Ex. A laser produces light with a wavelength of 650 nm and a power of 5 mW. How many photons per/s is it producing

$$\lambda = 650 \text{ nm} = 6.5 \times 10^{-7} \text{ m}$$

(convert to m!)

① First, find the energy

$$E = \frac{h\nu}{\lambda}$$

$$E = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{(6.50 \times 10^{-7} \text{ m})} = 3.06 \times 10^{-9} \text{ J}$$

② Divide the power with the energy

$$\frac{0.005 \text{ J/s}}{3.06 \times 10^{-9} \text{ J}} = 1.635 \times 10^{16} \text{ photons}$$

Kinetic energy of the ejected electron is calculated via conservation of energy:

$$E_{\text{light}} = E_{\text{binding}} + E_k$$

$$\therefore E_{\text{light}} = h\nu$$

E_{binding} : energy consumed in removing electron from its surface. This depends on the identity of the metal (how tightly the electrons are bound)

Ex. If an electron in a hydrogen atom were to be excited to the 3p orbital from the 2s orbital. How much energy?

$$\Delta E_{2s \rightarrow 3p} = -2.18 \times 10^{-18} \text{ J} \left(\frac{1}{n^2_{\text{final}}} - \frac{1}{n^2_{\text{initial}}} \right) \cdot Z^2$$

$$= -2.18 \times 10^{-18} \text{ J} \left(\frac{1}{9} - \frac{1}{4} \right) (1)$$

$$= 3.03 \times 10^{-19} \text{ J} \quad \leftarrow \text{energy required to excite an electron to the 3p orbital from 2s.}$$

Using the energy, you can determine the wavelength of light that is needed for the photon energy to absorb.

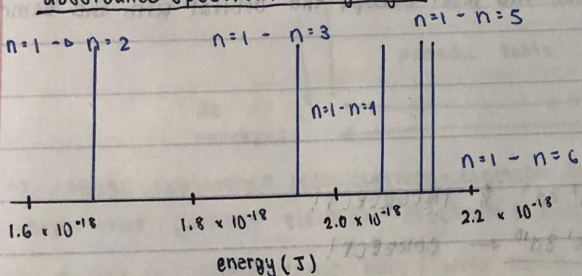
$$E = \frac{hc}{\lambda}$$

$$\lambda = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{(3.03 \times 10^{-19} \text{ J})} = 6.56 \times 10^{-7} \text{ m} \cdot \frac{1 \text{ nm}}{1.0 \times 10^{-9} \text{ m}} = 656 \text{ nm}$$

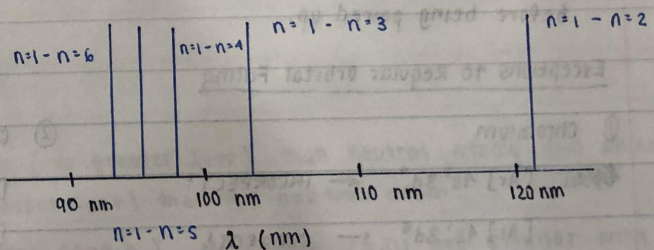
$$\lambda = \frac{hc}{E}$$

\therefore When a wavelength of 656 nm strikes a hydrogen atom, the photon energy will be absorbed to excite an e^- to the 3p orbital from 2s. This also means that the electron in a 3p orbital can emit light of wavelength 656 nm to relax to the 2s orbital.

absorbance spectrum of hydrogen



Wavelength scale of hydrogen



\therefore Energy increases as n transitions into higher levels but their wavelength becomes shorter

> when an electron is promoted to $n = \infty$. this means that the electron has been completely removed, aka. the ionization energy.

Ex. Calculate the ionization energy of ground state hydrogen.

$$(2.18 \times 10^{-18} \text{ J}) \left(6.02 \times 10^{23} \frac{\text{atoms}}{\text{mol}} \right)$$

$$= 1312360 \text{ J/mol} \cdot \frac{1.0 \times 10^{-3} \text{ kJ}}{1 \text{ J}} = \boxed{1.31 \times 10^3 \text{ kJ/mol}}$$

\leftarrow amount of energy to REMOVE an e^- .

> the product of the wavelength and frequency of light is a constant.

Why? $\rightarrow \nu = \frac{c}{\lambda}$

$\rightarrow \nu \cdot \lambda = c$
 \uparrow speed of light is $(3.00 \times 10^8 \text{ m/s})$, \therefore a constant

> if an e^- is added to an atom on the right side of the periodic table, it will feel a greater attraction to the nucleus b/c the ~~orb~~ orbital is lower in energy. (More energy released when added)

> noble gases have low electron affinities b/c it cannot accept more e^- .

> EA also ~~increases~~ ^{decreases} as the atom/ions ~~grow~~ grow bigger in atomic radii size b/c the orbital is further from nucleus.

Chapter 8

The Molecular Orbital and Valence Bond Theory:

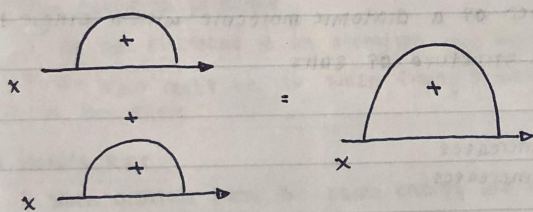
Main Idea: Combine the atomic orbitals to make new orbitals that give better descriptions to where electrons are in molecules.

Wave superposition: wave functions can be added / subtracted to produce new wave functions. The superposition changes the location of electron density, and can be used to form covalent bonds.

> forms covalent bonds when the waves superimpose and combine to produce a wave w/ larger or smaller amplitudes at certain points.

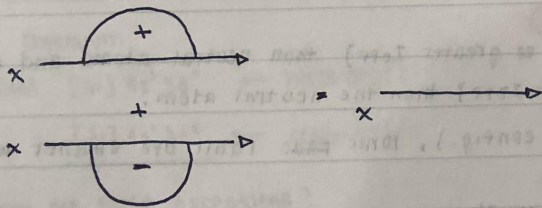
Molecular orbitals: bonding and anti-bonding

Bonding molecular orbital: formed from constructive interference and electron density is increased



=> constructive interference of the orbitals LOWERS energy

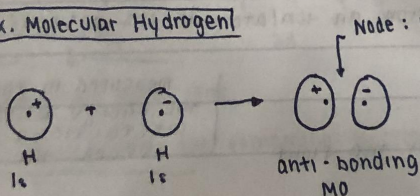
Anti-bonding molecular orbital: formed by two wavefunctions of different phases, there is destructive interference and the electron density is reduced.



=> destructive interference of the orbitals INCREASES energy

→ When orbitals have greater overlap, they have greater differences in energy between anti-bonding and bonding MOs.

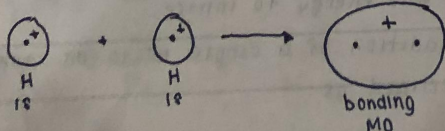
Ex. Molecular Hydrogen



Node: region where everything cancels out

=> the total # of MOs is always equal to the number of AOs interacting

=> when two ~~any~~ atomic orbitals (AO) are combined, the resulting ~~the~~ bonding MO will have fewer nodes than the ~~bonding~~ anti-bonding MO



=> the more Atomic ~~molecules~~ orbitals that overlap, the greater the energy gap

=> only atomic orbitals with same energy will interact significantly ($1s + 1s$), ($2s + 2p$)

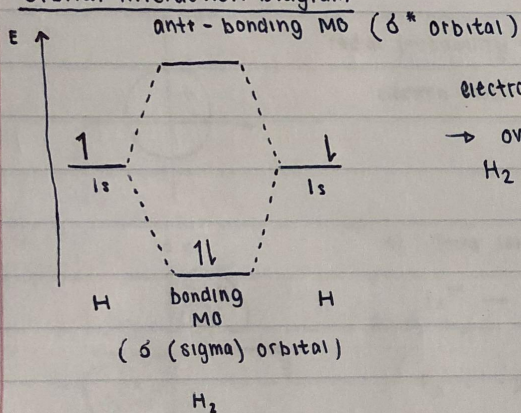
- * RMBR * ① the probability of finding an electron at a particular point is proportional to the wave function squared
 ② phase changes @ node and ③ probability of finding an e⁻ @ node is zero

Energy levels of Molecular Orbitals

Ex. H₂

- when the molecular orbitals are formed, the bonding MO is lower in energy relative to the 1s orbitals and the anti-bonding MO is higher in energy.

Orbital Interaction Diagram

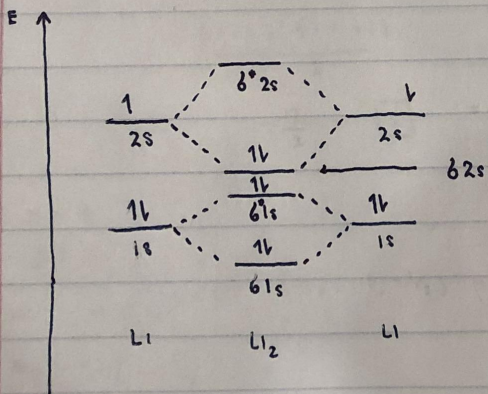


electronic configuration: $\sigma 1s^2$

→ overall energy of H₂ is lower than that of two H atoms, which is why H₂ is more energetically favoured

$$\text{Bond Order} = \frac{e_{\text{bonding}} - e_{\text{antibonding}}}{2} = \frac{2 - 0}{2} = 1 \text{ (single bond)}$$

Ex. 2 Li₂ (second row homonuclear diatomic species)



electronic config: $\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2$

$$\text{bond order} = \frac{4 - 2}{2} = 1$$

Chapter 7

The Effective Nuclear Charge: this applies to the electron-electron repulsion in multi-electron atoms.

For example in lithium, there are three electrons with two of them being closer to the nucleus. The third one, in the $2s$ orbital, is essentially being shielded by the electrons in the $1s$ orbital from feeling the full $+3$ charge from the nucleus.

The approximation of the Z_{eff} is $Z - S$, Z = atomic number, S = shielding electrons

4th quantum number: spin quantum number (m_s)

$$m_s = +\frac{1}{2} \text{ (spin up "↑")}$$

$$m_s = -\frac{1}{2} \text{ (spin down "↓")}$$

Electron Filling Rules

① Aufbau principle (building up principle)

> must fill the orbitals with the lowest energy first

② Pauli exclusion principle

> no two electrons in an atom/ion may have the same four quantum numbers (n, l, m_l, m_s)

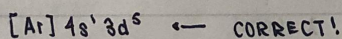
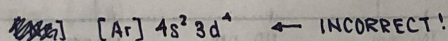
> the spin must be $\uparrow\downarrow$ when filling orbitals, not $\uparrow\uparrow$ or $\downarrow\downarrow$ b/c this means the spin quantum number is the same

③ Hund's Rule

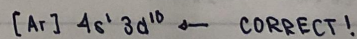
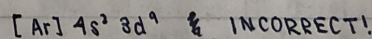
> when orbitals have the same energy are available, electrons must occupy the orbital with the same spin before being paired up.

Exceptions to Regular Orbital Filling

a) ① Chromium

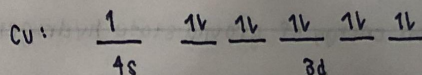
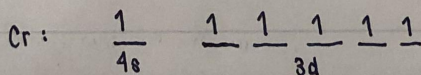


② Copper



* Why are these exceptions?

> More stable having two half-filled shells / one half-filled and one filled shell

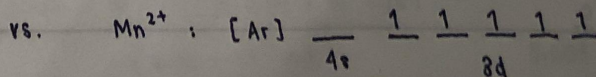
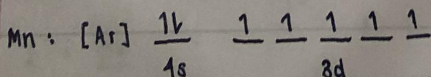


b) Transition metal ions

→ when ionized, the remaining electrons are found in the d-subshell

Ex. manganese

manganese (II)

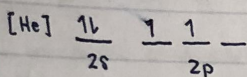


(this is considered the ground state for Mn^{2+} !)

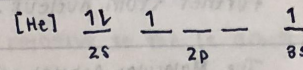
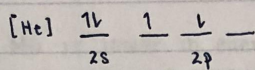
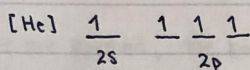
Ground state: the electronic configuration resulting from following all electron filling rules, with the exceptions of chromium, copper, and the transition metal ions.

> if a species violates Hund's Law and/or the Aufbau principle, it is considered an excited state.

Ex. Carbon



ground state



examples of excited states for carbon

Magnetic properties

> the "spins" in the orbital relates to the magnetic properties of a species. if there are unpaired electrons, the species will possess an overall magnetic moment.

paramagnetic: species w/ one or more unpaired electrons

diamagnetic: species w/ no unpaired electrons

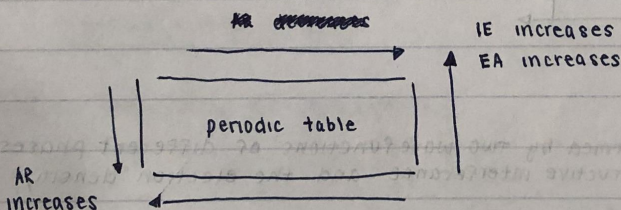
periodic properties

① Atomic and Ionic radii: three ways to measure the size

i) covalent: measured as half the homonuclear distance of a diatomic molecule with a single bond

ii) ionic: estimated measured from the crystal lattice structure of salts

iii) van der Waals: distance between non-bonded atoms



→ cations experience less electron-electron repulsion (so greater Z_{eff}) than neutral atoms and anions experience greater electron-electron repulsion (less Z_{eff}) than the neutral atom.

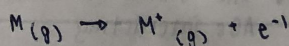
→ a set of isoelectronic ions (with same electronic config.), ionic radii are smaller with increasing Z .

Ex. a set of isoelectronic ions: O^{2-} , F^- , Na^+ , Mg^{2+} → all w/ $10 e^-$

⇒ O^{2-} has largest radii b/c it has the smallest Z compared to F , Na , and Mg .

② Ionization Energy: the energy required to remove a single e^- from an ion/atom in its gaseous state

First ionization process of general atom, M is described as:



> since the valence orbitals are closer to the nucleus in atoms of the right side of the table, it will require more energy to be ionized.

> electrons are more tightly held in atoms w/ smaller radii → more energy to ionize.

measured in gas phase b/c the energy between interactions will not affect the measurement

③ Electron Affinity: the energy change that results from the addition of a single e^- to an atom or ion.

ionization of a general atom, M , to its anionic form is described as:

