

Atomic Structure and Periodicity: Patterns

Inspired by Paul Groves

A BLUFFER'S GUIDE

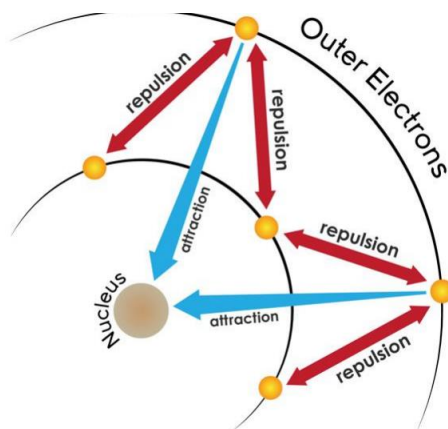
- $c = v \lambda$
 c = speed of light = 3.00×10^8 m/s
 v = frequency in hz, sec^{-1}
 λ = wavelength in meters
- $E = hv$
 E = energy in Joules, kgm^2/s^2
 h = Planck's constant 6.626×10^{-34} Js
 v = frequency in hz, sec^{-1}
- Long wavelength
 = low frequency
 = low energy
- Short wavelength
 = high frequency
 = high energy
- de Broglie Equation

$$\lambda = \frac{h}{mv}$$
 m = particle mass
- Bohr Equation

$$E = -2.178 \times 10^{-18} \text{J} \left(\frac{Z^2}{n^2} \right)$$
 Z = nuclear charge n = energy level
- Energy change between two levels

$$-2.178 \times 10^{-18} \text{J} \left(\frac{Z^2}{n_{\text{final}}^2} - \frac{Z^2}{n_{\text{initial}}^2} \right)$$

**doesn't usually show up on AP Exam*
- Shielding – electrons are simultaneously attracted to the nucleus and repelled by each other.



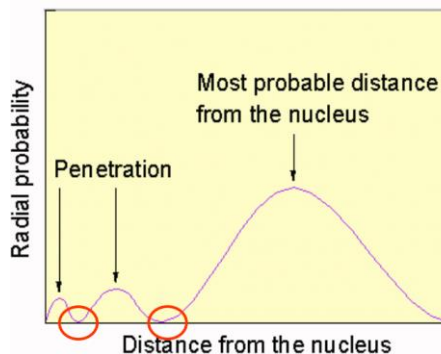
- The repulsion results in less attractive force between outer electrons and the nucleus.

Outer electrons are shielded by the core, inner electrons. Outer electrons do not effectively screen for each other since they are in the same level.

Shielding causes outer electrons to not experience the full strength of the nuclear charge. The electrons would be more attracted to the nucleus if the electrons were not there!

- Trend in shielding strength:
most $s > p > d > f$ *least*
- Effective nuclear charge – a net positive charge that is attracting a particular electron

$$Z_{\text{effective}} = Z - S$$
 Z = nuclear charge (number of protons)
 S = number of electrons in lower energy levels
**Note – this is oversimplified a lot!*
- Penetration – when an e^- spends time closer to the nucleus than its outer boundary.



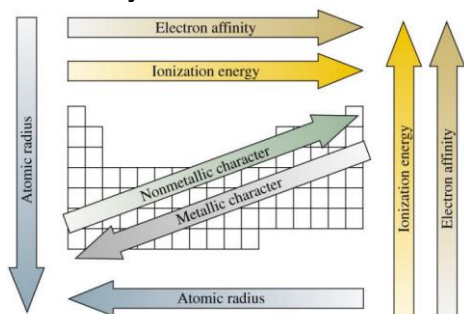
**nodes are areas with zero probability*

The closer the electron is to the nucleus, the more attraction it experiences.
 The more e^- penetrates = more attraction

- Trend in penetration towards nucleus:
most $s > p \gg d > f$ *least*

14. Shielding and penetration explain a lot of things! Z_{eff} , Ionization Energies, exceptions to patterns on periodic table etc

15. Summary of Periodic Trends:



16. Careful with phrasing your answers! Remember...AP Chem loves “columbic attraction” type explanations!

17. **Two elements in the same period?**

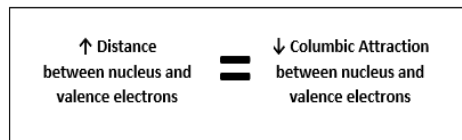
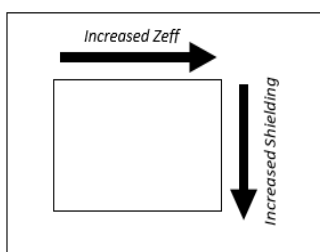
Discuss the fact that...

- Each element has valence electrons that are located in the same energy level.
- One atom has a greater number of protons (greater nuclear charge).
- More protons results in a stronger attraction between the nucleus and the valence e^- s
- Stronger columbic attraction between nucleus and valence e^- s results in a smaller atomic radius.
- That is what “Greater Effective Nuclear Charge” is trying to explain!

18. **Two elements in the same group?**

Discuss the fact that...

- Valence e^- s are not located in the same energy levels, one has more principal energy levels.
- Valence e^- s for one element are in a higher energy level than the valence e^- s of the other element.
- The e^- s in the higher energy level are (on average) located farther away from nucleus.
- Being further away from the nucleus results in a weaker attraction btwn the nucleus and valence e^- s
- Weaker columbic attraction btwn nucleus and valence e^- s results in a larger atomic radius.
- Increased e^- s also results in more repulsions btwn e^- s resulting in a larger atomic radius
- That’s what “Increased Shielding” is trying to explain!



- Everything Comes Down to...
- Attractions
 - Repulsions
 - Energy

19. Ionic Radius Trend:

Cation < Neutral version of itself
Anion > Neutral version of itself
Cations < Anions

Isoelectric – same electron configuration
Larger (+) charge = smaller cation
protons pulling on fewer electrons
Larger (–) charge = larger anion
protons pulling on more e^-

20. Irregularities in patterns

Extra repulsions of e^- s in paired orbitals

- Makes it easier to remove an e^-
 - Lower IE than expected
- Moving to a p orbital (Mg → Al)
 - p orbital does not penetrate as much as an s orbital does
 - Less nuclear attraction
 - Lower IE than expected

21. Large jump in IE shows when you begin removing core electrons:

Element	IE ₁	IE ₂	IE ₃	IE ₄	IE ₅	IE ₆	IE ₇
Na	496	4560					
Mg	738	1450	7730				
Al	578	1820	2750	11,600			
Si	786	1580	3230	4360	16,100		
P	1012	1900	2910	4960	6270	22,200	
S	1000	2250	3360	4560	7010	8500	27,100
Cl	1251	2300	3820	5160	6540	9460	11,000
Ar	1521	2670	3930	5770	7240	8780	12,000

22. Electronegativity differences between bonded atoms results in a molecule being polar or nonpolar:

- Pure covalent = EN difference of 0
 - Nonpolar covalent = EN diff. of 0.1 – 0.4
 - Polar covalent = EN diff. of 0.5 – 1.9
 - Ionic = EN diff. larger than or equal to 2.0
- *ranges can vary, calculations rarely appear*

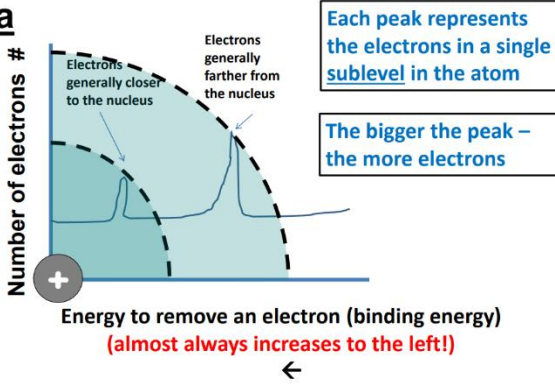
23. Magnetic properties are a result of how the electrons are arranged in orbitals

- Paramagnetic – net magnetic field, unpaired electrons in orbitals, weakly attracted by a magnet.
- Diamagnetic – no net magnetic field, all paired electrons in orbitals, weakly repelled by a magnet

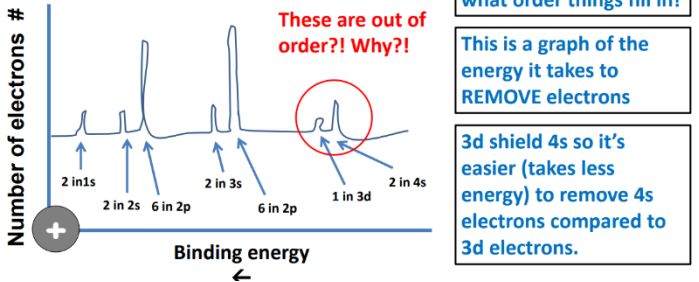
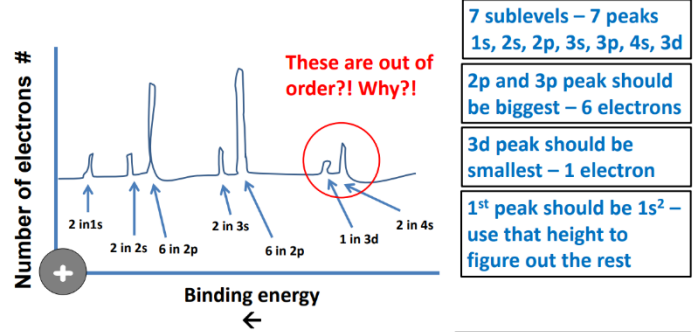
24. Photoelectron Spectroscopy (PES)

PES Data

A graph!



Scandium ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$)

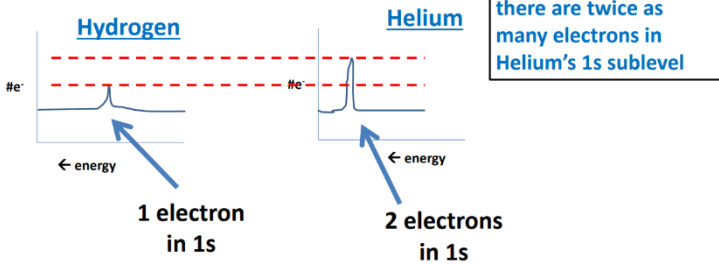


This is NOT a graph of what order things fill in!

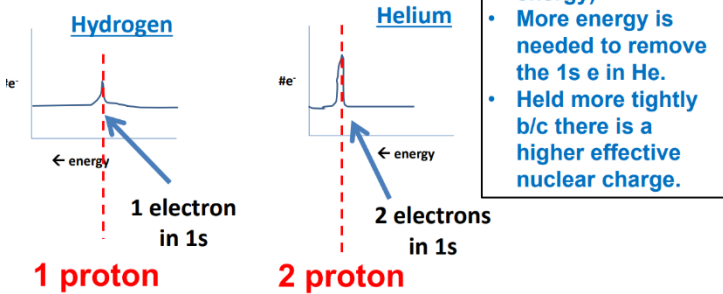
This is a graph of the energy it takes to REMOVE electrons

3d shield 4s so it's easier (takes less energy) to remove 4s electrons compared to 3d electrons.

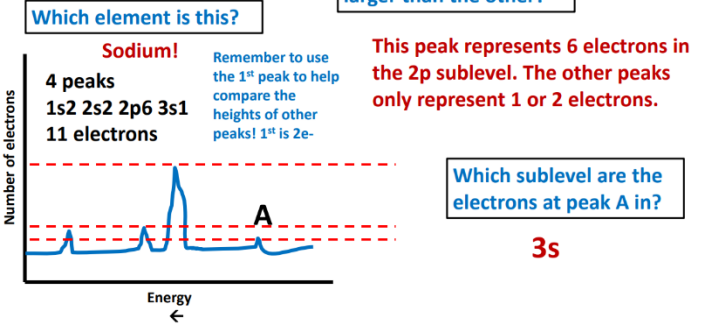
Hydrogen vs. Helium



Hydrogen vs. Helium



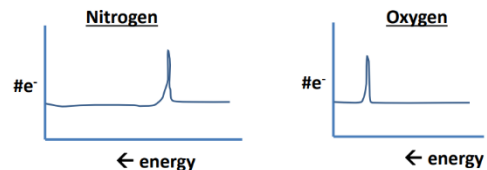
Example #1



Example #2

The PES data above shows only the peak for the 1s electrons. Why is the peak for Nitrogen farther to the right?

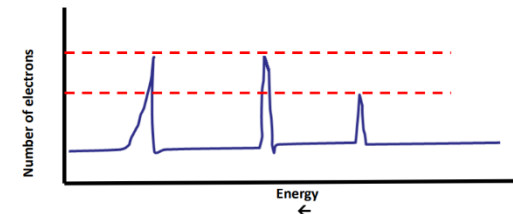
It takes less energy to remove a 1s electron from Nitrogen because it has a larger radius than Oxygen (because it has a lower Effective nuclear charge (less protons) than oxygen) so there is less attraction between the nucleus and the electron in Nitrogen than in Oxygen.



Example #3

Draw the expected PES Spectrum for the element boron

1. Write configuration – $1s^2 2s^2 2p^1$
2. Figure out how many peaks – 3
3. Sketch 1s² peak first – use that to figure out sizes of all other peaks



Oxygen – $1s^2 2s^2 2p^4$

