Spectroscopy

Spectroscopy: a study of the interaction between matter and electromagnetic radiation

- Can be used to determine the atoms, molecules, or structure of a given substance
- So many kinds!!

Types of Spectroscopy

Name of Spectroscopy	Type of Radiation Used	Relative energy	What does it do to the atom/molecule?	What does it tell us?
Photoelectron spectroscopy (PES)	X-ray	very high	Removes electrons (valence and core).	• Identity of element • How tightly electrons are held by the nucleus
UV-Visible spectroscopy (UV-Vis)	Ultraviolet (UV)	high	Excites electrons to jump between energy levels.	• Identity of element or molecule
UV-Visible spectroscopy (Colorimetry)	Visible	medium		• Identity of element or molecule • Concentration of solution
IR (vibrational) spectroscopy	Infrared (IR)	low	Changes vibrations within bonds.	• Types of atoms, bonds, and functional groups within a molecule
Microwave (rotational) spectroscopy	Microwave	very low	Changes the rotation of atoms in bonds.	• Location of hydrogen atoms within a molecule

Photoelectron Spectroscopy (PES)

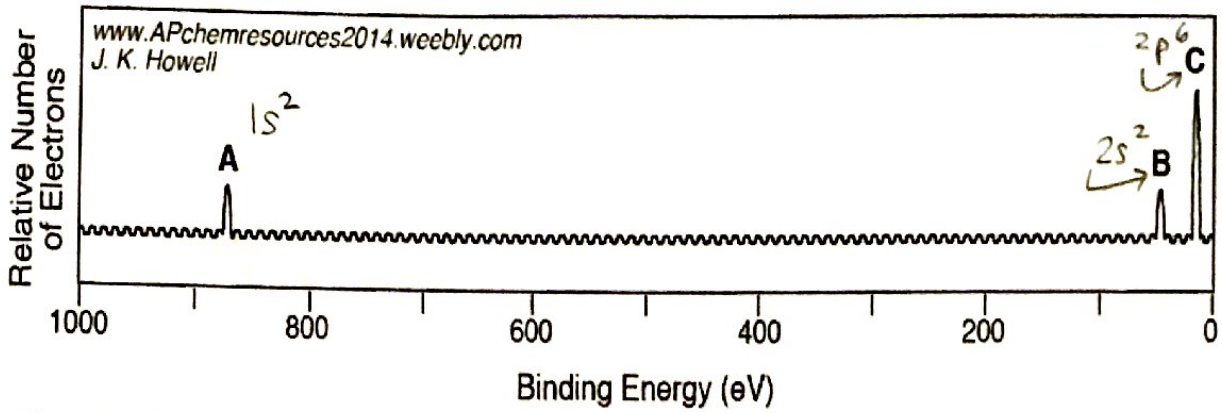
Photoelectron Spectroscopy (PES): a technique to determine the ionization (or binding) energy of EVERY electron in an atom

- Ionization energy (for PES, more commonly referred to as the **binding energy**): the energy required to remove (ionize) an electron from an atom
- Binding energy is plotted on the horizontal axis, with energy decreasing (!!) from left to right (although sometimes this is flipped, so always check)

How to Interpret PES Spectra

- Peak **height** corresponds to the relative # of electrons in each sublevel of an atom
- Peak **location** corresponds to the relative amount of energy required to remove each electron
  - Higher energies = sublevels found closer to the nucleus (1s, 2s, etc)
  - ~~Higher~~ Lower energies = sublevels found farther from the nucleus
- When comparing PES from different atoms:
  - As the number of protons in the nucleus increases, the binding energy will ↑ for electrons in comprable sublevels
  - As the number of e⁻ in a specific sublevel increases, the peak height will ↑ for electrons in comprable sublevels

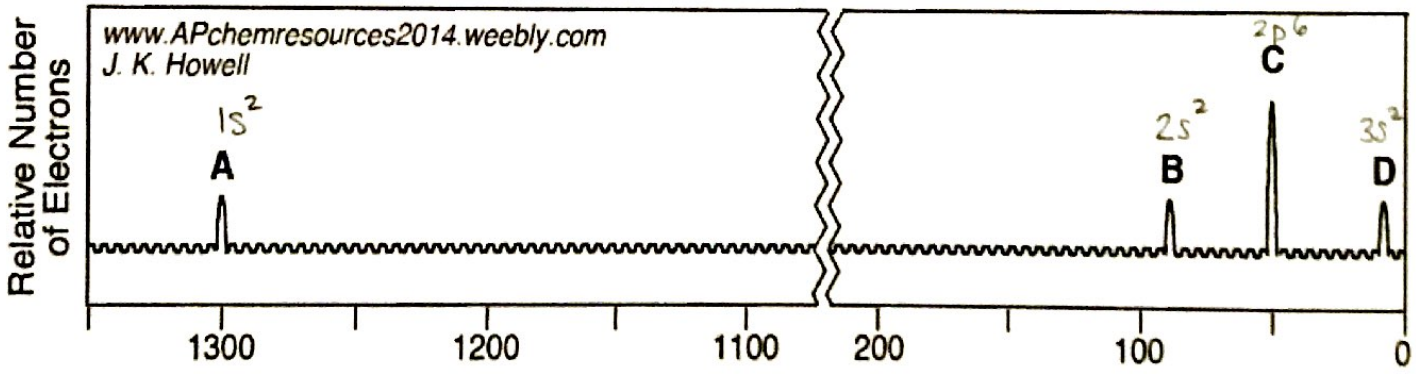
Photoelectron Spectrum of Neon



Interpretation of Spectrum:

- Electrons in 1s subshell (peak A) have a much higher binding energy than electrons in 2s (peak B), because the core electrons experience a much higher effective nuclear charge than valence electrons.
- The 2p signal (peak C) is three times higher than the 1s (peak A) and 2s (peak B) signals, indicating it contains triple the number of electrons ($2p^6$ vs $1s^2$, $2s^2$).

Photoelectron Spectrum of Element Z



1. What is the identity of element Z?

   a. Boron b. Carbon c. Neon (d.) Magnesium

2. Label the identity of each peak with principal quantum number, n (energy level), subshell (s, p, d, or f) and a superscript representing the number of electrons found in the subshell.

3. If the PES spectrum above had actually represented the element sodium, what would be different? List at least two differences you would expect to see:

   - lower binding energies ($Mg = 12\ p^+$, $Na = 11\ p^+$)
   - 3s peak $\frac{1}{2}$ height (only 1 e^- instead of 2 e^-)
     Na Mg