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603  
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## Electronic Structure of Atoms

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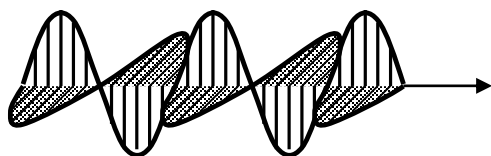
*AP Chemistry Lecture Outline*

electronic structure: the arrangement of electrons in an atom

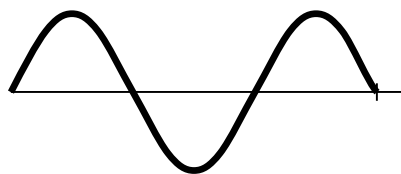
quantum mechanics: the physics that correctly describes atoms

### electromagnetic radiation (i.e., light)

- waves of oscillating electric (E) and magnetic (B) fields
- source is...



### Characteristics of a Wave



frequency: the number of cycles per unit time (usually sec)

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electromagnetic spectrum: contains all of the “types” of light that vary according to frequency and wavelength

- radio, microwaves, infrared, visible, ultraviolet, X rays, gamma rays, cosmic rays

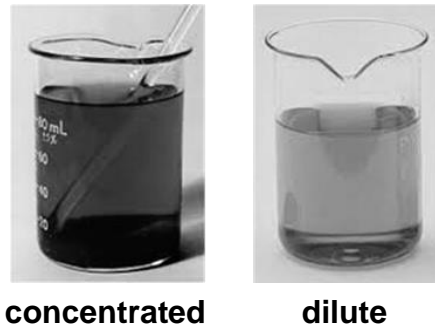


- visible spectrum ranges from only ~400 to 750 nm (a very narrow band of spectrum)

Video  
606  
(8:07)

Light (in all its forms) is employed to analyze matter.

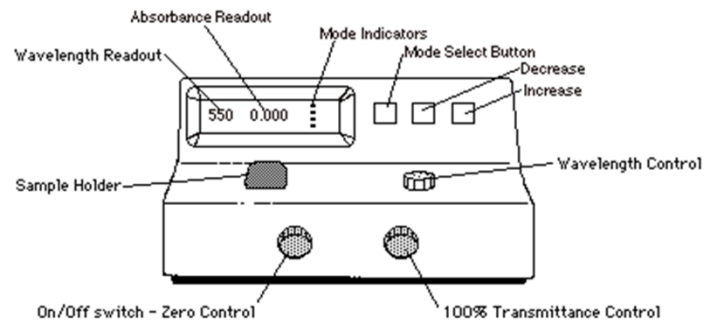
We know intuitively something about the concentration of a solution just by its visual appearance.



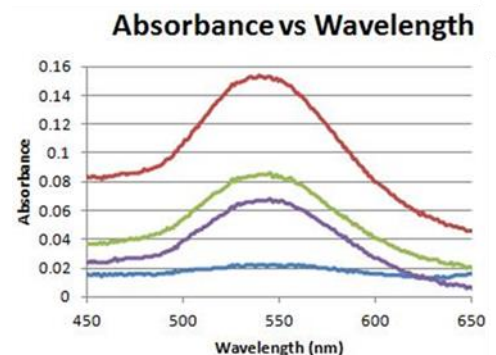
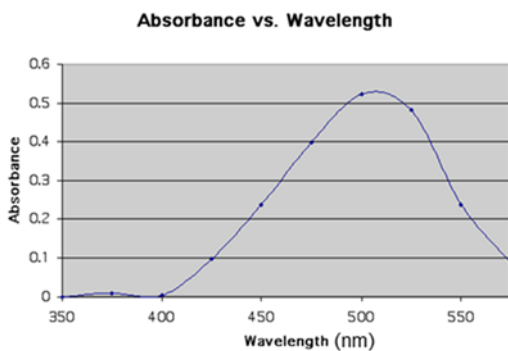
When light of a specific wavelength is directed at a colored solution, some of the photons are absorbed and some are transmitted.



### Using a Spectrophotometer to Determine an Unknown Solution Concentration

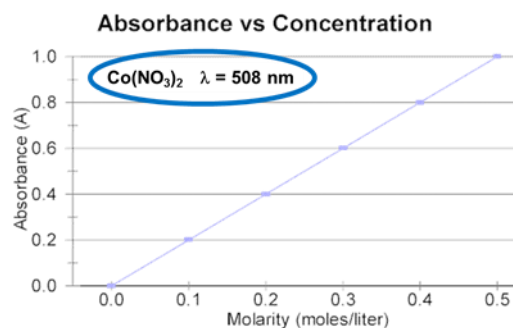


1. Learn to use a spectrophotometer.
2. Using a soln of your analyte of known conc., choose various  $\lambda$ s on your spectrophotometer, record the Abs for each, and make an Abs vs.  $\lambda$  graph.



3. From the graph, choose the  $\lambda$  for which Abs is maximized.

- Using several known solns of your analyte and your chosen  $\lambda$ , record the absorbance reading for each soln, and make a graph of Abs vs. concentration.
- Finally, place a cuvette with your unknown soln into the spectrophotometer, record the absorbance, and go to your Abs vs. concentration graph to determine your unknown concentration.



Video  
609  
(8:35)

### Beer's Law

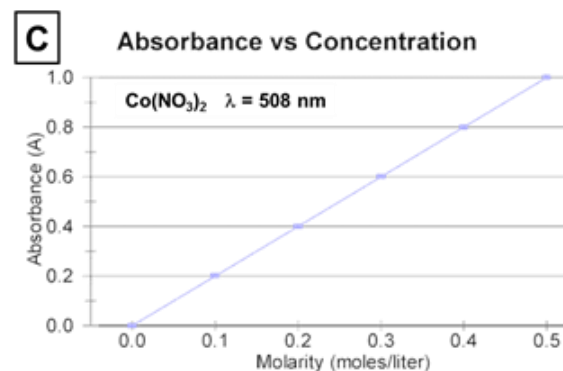
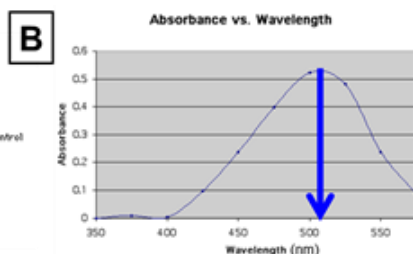
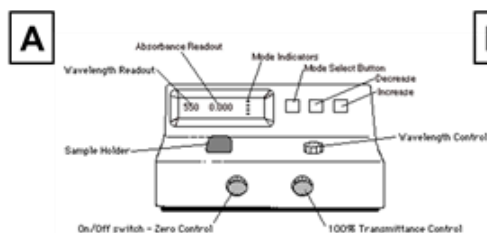
Beer's law (or the Beer-Lambert law) relates the absorbance of a soln to its concentration:

- Abs = absorbance
- $e/A$  = molar absorptivity
- $L/t$  = path length
- $c/M$  = soln molarity

light source  
(specific  $\lambda$ )



light  
detector



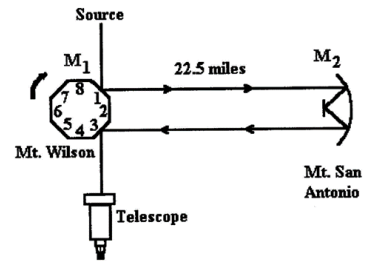
- EX. For a given analyte at the max. Abs  $\lambda$  of 425 nm, a 0.42 M soln produces an Abs of 0.13. Using Beer's law, determine the conc. of a solution whose Abs is 0.074 under the same experimental conditions.

Video  
612  
(8:14)

The speed of light in a vacuum  
(and in air) is constant: -- Equation:

In 1900, Max Planck assumed that energy can be absorbed or released only in certain discrete amounts, which he called quanta. Later, Albert Einstein dubbed a light "particle" that carried a quantum of energy a photon.

-- Equation:



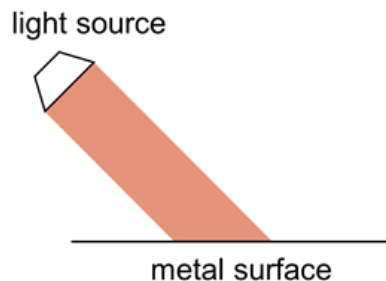
**Michelson's experimental setup**

EX. A radio station transmits at 95.5 MHz (FM 95.5). Calculate the wavelength of this light and the energy of one of its photons.

Video  
615  
(5:39)

In 1905, Einstein explained the photoelectric effect using Planck's quantum idea.

-- only light at or above a threshold freq. will cause  $e^-$  to be ejected from a metal surface



Einstein also expanded Planck's idea, saying that energy **exists** only in quanta. Light has both wavelike and particle-like qualities, and...

Video  
618  
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### Photoelectron Spectroscopy (PES)

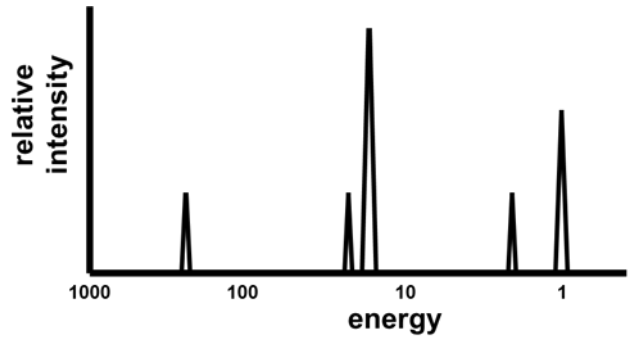
Photoelectron or (photoemission) spectroscopy (PES) employs the photoelectric effect to measure the binding energies of  $e^-$  in

\*\* PES data is...

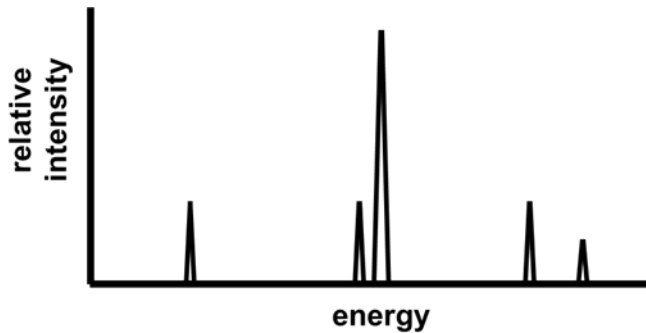
atoms. The data is most commonly communicated in graphical form.

### How to Read a PES Graph:

- 1.
- 2.



EX. Determine the element represented by the following PES graph.



EX. Draw an approximate PES graph for chlorine.

Video  
621  
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### Line Spectra

Ordinary white light is dispersed by a prism into a...

From the gas in a nearly-evacuated gas-discharge tube, we instead get a...

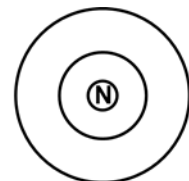


Video  
624  
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Niels Bohr took Planck's quantum idea and applied it to the  $e^-$  in atoms.

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planetary  
(Bohr)  
model



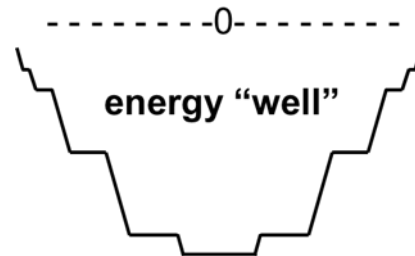
-- Bohr assumed that the  $e^-$ 's in his circular orbits had particular energies, given by:

$$R_H = \text{Rydberg constant} = 2.18 \times 10^{-18} \text{ J}$$

$n = 1, 2, 3, \dots$  (the principal quantum number)

The more/less (–) an electron’s energy is...

When  $n$  is very large,  $E_n$  goes to zero, which is the most energy an  $e^-$  can have because...



- Bohr stated that  $e^-$  could move from one level to another, absorbing light of a particular freq. to “jump up” and releasing light of a particular freq. to “fall down.”
- Bohr’s model (i.e., its specific equation) worked only for atoms with...

Video  
627  
(5:22)

Find the wavelength, frequency, and energy of a photon of the emission line produced when an  $e^-$  in a hydrogen atom makes the transition from  $n = 5$  to  $n = 2$ .

Video  
630  
(4:32)

### The Wave Behavior of Matter

Since light (traditionally thought of as a wave) was found to behave as both a wave and a particle, Louis de Broglie suggested that matter (traditionally thought of as particles) might also behave like both a wave and a particle. He called these...

- The wavelength of a moving sample of matter is given by:

EX. A proton moving at 1200 m/s would be associated with a matter wave of how many nm?

Video  
633  
(6:28)

A wave is smeared out through space, i.e., its location is not precisely defined. Since matter exhibits wave characteristics, there are limits to how precisely we can define a particle's (e.g., an e<sup>-</sup>'s) location.

- the limitation also applies to a particle's...
- Heisenberg's uncertainty principle:

Video  
636  
(4:28)

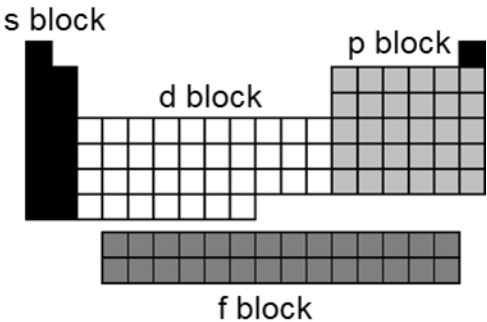
Schrodinger's wave equation (1926) accounts for both wave and particle behaviors of e<sup>-</sup>.

- Solutions to the wave equation yield wave functions, symbolized by  $\Psi$ , which have no physical meaning, but  $\Psi^2$  at any point in space gives the probability that you'll find an e<sup>-</sup> at that point.  $\Psi^2$  is called the probability density, which gives the electron density.
- Orbitals describe a specific distribution of electron density in space.  
Each orbital has a characteristic shape and energy.

Video 639 (11:13)

**Electron Configurations:** Where are the e<sup>-</sup>? (probably)

- H
- He
- P
- Fe<sup>3+</sup>



Aufbau Principle:  $e^-$  will take the lowest-energy orbital that is available

$Al^{3+}$

$O^{2-}$

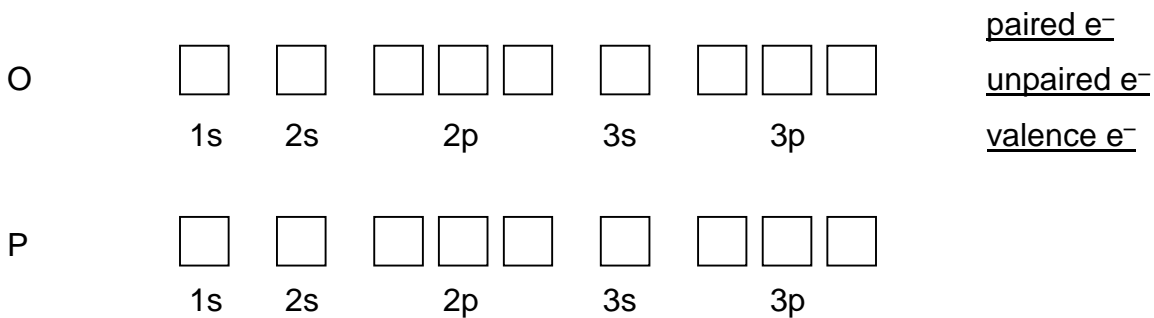
isoelectronic species:

$F^-$

$N^{3-}$

Hund's Rule: each degenerate orbital must have one  $e^-$  before any take a second

**Orbital Diagrams**...show spins of  $e^-$  and which orbital each is in



**Shorthand Electron Configuration (S.E.C.)**

1. Put symbol of noble gas that precedes element in brackets.
2. Continue writing  $e^-$  config. from that point.

S

Co





Video  
648  
(12:04)

Quantum numbers are used to describe where an  $e^-$  is in an atom.

1. principal quantum number,  $n$  ( $n = \text{integers } 1, 2, 3, \dots$ )
  - correspond to the energy level of the electrons
  - All orbitals having the same  $n$  are called an electron shell (e.g., 2s and 2p).
2. angular momentum quantum number,  $l$  ( $l = \text{integers from } 0 \text{ up to } (n - 1)$ )
  - This number defines the type of subshell:
  - For a given shell, the energies of orbitals go:
3. magnetic quantum number,  $m_l$  ( $m_l = \text{integers from } -l \text{ to } l$ )
  - describes the orientation of an orbital in space
  - You should know the shapes and orientations of the s, p, and d orbitals:  
s,  $p_x$ ,  $p_y$ ,  $p_z$ ,  $d_{yz}$ ,  $d_{xz}$ ,  $d_{xy}$ ,  $d_{x^2-y^2}$ ,  $d_{z^2}$
4. electron spin quantum number,  $m_s$ 
  - only two values:  $+\frac{1}{2}$  or  $-\frac{1}{2}$  ("spin-up" and "spin-down")
  - Pauli exclusion principle: No two electrons in an atom may have the same set of four quantum numbers (i.e., an orbital may hold only two electrons, and they must have opposite spins).

EX. What are the values of  $n$  and  $l$  for the following sublevels?

2s

3d

4p

5s

4f

EX. Write the possible sets of the four quantum numbers for a 4p electron.

Write the four quantum numbers of each of the six 3d electrons of an iron atom.