Slide 1

Learning in general:

1. Read ahead form the book and the Powerpoint slides.
2. Print out the slides. You should never need to copy what is on the projector. You should be annotating what is on the slides based on our discussion.
3. When doing problems, write out what you are doing. Just punching numbers into the calculator is not the way to learn to do a problem.
4. You should look at the homework in advance of class and deadlines.

Slide 2

Learning in general:

The best strategy is: read ahead and try a problem, come to lecture (with the notes printed) and ask questions about your reading or what I'm doing in class, review the notes and do the homework.

Slide 3

Electronic Structure of Atoms

Chemistry is Electrons

Slide 4

What's this thing called light?

Light is an oscillating electromagnetic wave!

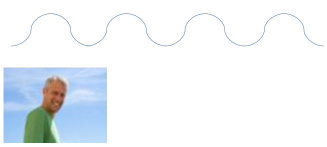
There are two ways to look at any wave:

A) Freeze the wave and walk along it.

B) Stay put and watch the wave go by.

Slide 5

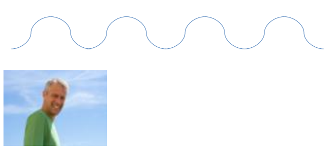
Freeze the wave and walk…



Slide 6

What do I see on my walk?

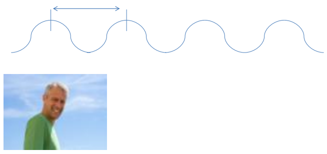
The wave going up and down and up and down and up and down and up and down and…



Slide 7

What do I see on my walk?

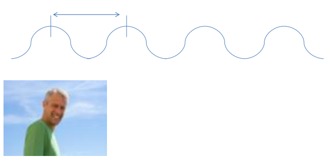
The distance between two peaks is called the wavelength: how far I walked!



Slide 8

What do I see on my walk?

Wavelength is abbreviated as λ



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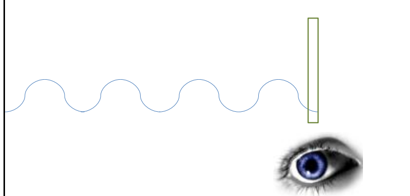
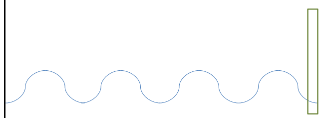
What if instead of walking I sit still and let the wave go by…



Slide 10

I see it go up and down and up and down…



The number of times it goes up and down in a second (or minute or hour or day…) is called its frequency and this is abbreviated ν (Greek letter "nu")

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Wavelength and frequency are related…

…just look at the units.

What's the unit of wavelength?
Meters (or the equivalent)

What's the unit of frequency?
#/sec (or the equivalent)

Slide 12

What do you get when you combine distance and time?

VELOCITY!!!

Miles per hour
Meters per second
Kilometers per day

Slide 13

$\lambda\nu=c$

Where c is the speed of light.

The speed of light is actually constant in vacuum and has a value of $2.997x10^8$ m/s or ($3.00 x10^8$ m/s)

Why constant in vacuum?

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No molecules in a vacuum…

If the light keeps bumping into molecules, it slows it down!

Air is actually pretty close to vacuum (at least to 3 sig figs) and we use the same value in air.

Slide 15

What is the frequency of 600 nm orange light?

$c=\lambda\nu$

$c=3.00x10^8$ m/s (in vacuum)

$3.00x10^8$ m/s = 600 nm * ν

UNITS! UNITS! UNITS!

$3.00x10^8 \text{ m/s} = 600 \text{ nm} * \frac{10^{-9} \text{ m}}{\text{nm}} * \nu$

$\nu = \frac{3.00x10^8 \text{ m/s}}{600x10^{-9} \text{ m}} = 5 \times 10^{14} \text{ 1/s} = 5x10^{14} \text{ Hz}$

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Boy, I need a few more slides here…

The energy contained in a beam of light was actually a source of confusion.

In our everyday experience, a 1000 W light bulb is much hotter than a 25 W light bulb…no matter what color it is!

Why is it hotter?
It has more energy!

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But why does it have more energy?

It has more energy because it has more light waves in it NOT because the light waves are bigger.

Think of the ocean and compare a tsunami to a million ripples…

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When light strikes matter…

What happens? Or what COULD happen?

1. It bounces off.
2. It goes right through.
3. It gets absorbed.

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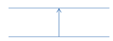
Absorbed light

Absorbing light becomes a means of probing matter.

When light is absorbed it must be tuned to the energy difference between two states.



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Different wavelengths of light interact with different things:

Infrared light (longer than 700 nm) interacts with the vibrations of bonds.

Microwave light (even longer wavelengths) interact with rotations of bonds.

Visible (400-700 nm) or ultraviolet (shorter than 400 nm) interact with the electrons.

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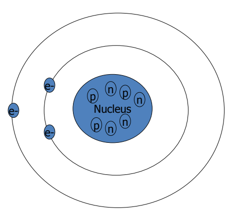
The Bohr Model and the Photoelectric effect.



Absorbing UV or visible light moves the electrons to a higher electron state.

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Bohr model and the photoelectric effect.

What if you absorb a LOT of energy? So much so that there are no more orbitals for the electron to go into?

The electron is knocked out of the atom! This is called the "photoelectric effect".

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Tsunami or a million ripples…

Suppose I need 10^{-18} J of energy to knock an electron off. This is called the work function of a material: the smallest amount of energy that will cause an electron to be emitted.

If I need 10^{-18} J of energy, where am I going to get it?

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I'm an atom and I need an Eve…

My work function is 10^{-18} J. Can I get the energy from:

A) A 10^{-18} J light bulb (white light)
B) 10 light waves with 10^{-18} J
C) A single light wave with 10^{-18} J of energy
D) A 100 W light bulb (100 J/s)
E) All of the above

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All of the above seems correct…

…so it isn't.

It turns out that light energy is not additive in the way that normal heat is. It comes prepackaged in single waves called "photons" where the energy of each photon is related to its frequency (or wavelength).

Slide 26

Enter Planck and his constant

$$E = h\gamma$$

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

h=Planck's constant = 6.626×10^{-34} J s

Slide 27

How much energy does a 600 nm orange photon possess?

$E = h * \nu$

$h = 6.626 \times 10^{-34}$ Js

$E = 6.626 \times 10^{-34}$ Js * 5×10^{14} s^{-1}

$E = 3.313 \times 10^{-19}$ J in a single photon

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Total energy in a beam of light?

Like all energy, the energy in a beam of light should be the sum of the energies of each little wave of light.

So, if you take four 600 nm photons, the total energy is:

4* 3.313×10^{-19} J = 1.33×10^{-18} J

That should be enough to knock my electron off!

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Damn electron won't leave!

But if you shine four 600 nm photons with a total energy of 1.33×10^{-18} J onto a material with a work function of 10^{-18} J no electron is emitted!!!

In fact if you have a 100 W 600 nm light bulb and shine it on the surface for an hour, the surface will be exposed to 360,000 Joules of energy and not a single electron will be emitted.

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This is quantization.

In order for an electron to make the jump it must have a landing pad. Only photons with the correct energy can be absorbed.

Or, as we scientists say, no halvesies!

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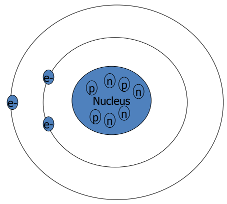
You must tune the energy to the energy separation between orbitals.



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Chemical Reactivity

The nucleus is encased in electrons.

The nucleus is stable and unchanged in chemical reactions.

When 2 atoms meet, it is their electrons that bump together.

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Chemical Reactivity…

…is all about the electrons.

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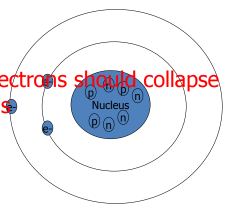
Electronic Structure of Atoms

Since the electrons are so important, understanding the electronic structure of atoms is critical to understanding why atoms react with each other.

The first thing we need to do is move beyond classical physics and the Bohr Model

Slide 35

What's wrong with the Bohr Model?



The electrons should collapse into the nucleus

Slide 36

It doesn't ☺

The electron "orbits" are stable and electrons can move between them by absorbing light (higher energy orbitals) or emitting light (moving into lower energy orbitals).

Slide 37

It's CSI!

The absorption and emission of light are characteristic of the materials.

The energy of the transition is just:

$\Delta E = E_{final\ state} - E_{initial\ state}$

The math gets complicated in a hurry…

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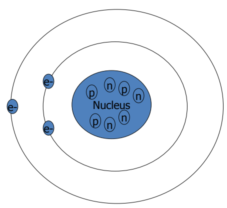
It's just charge to charge attraction…



BUT…there's also charge to charge repulsion….

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Anything beyond hydrogen…

…becomes hard to come up with a simple algebraic relationship.

$$\Delta E = \frac{hc}{\lambda} = Rhc\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

Where $R=1.097\text{x}10^{7}\ m^{-1}$ is the "Rydberg constant" and m and n are the initial and final orbitals.

$$\frac{1}{\lambda} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

Slide 40

Quantum electronic structure

The solution to the electron paradox is that the world of the atom is not “classical” but “quantum mechanical”.

In a quantum world, only certain discrete energy levels are allowed. You cannot slowly decay in orbit until you crash into the nucleus.

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Electron Orbitals

- Electron orbitals are diffuse. The electron is not a hard little pellet, but a “probability cloud”.
- Electron orbitals are 95% probability intervals.
- Allowed electron orbitals are determined by 4 quantum numbers.

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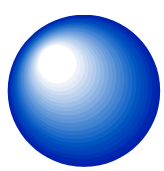
Electron Orbitals



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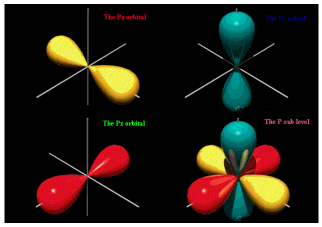
p-orbital



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Electron Orbitals

- Every electron is represented by 4 quantum numbers. These electron Quantum numbers are:

n = principal quantum number (kind of like the Bohr orbit)

l = angular momentum quantum number

m_l = magnetic quantum number

m_s = spin quantum number

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Allowed Quantum numbers

n = 1, 2, 3, 4, 5….

l = 0, 1, 2, 3, 4…(n-1)

m_l = -l, -l+1…-1, 0, 1…l-1, l

m_s = -1/2, ½

Notice that l depends on n and m_l depends on l

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Possible Quantum numbers

n = 1, l=0, m_l = 0, m_s=-1/2

n = 1, l=0, m_l = 0, m_s=+1/2

n = 2, l=0, m_l = 0, m_s=-1/2
n = 2, l=0, m_l = 0, m_s=+1/2

n = 2, l=1, m_l = -1, m_s=-1/2
n = 2, l=1, m_l = -1, m_s=+1/2
n = 2, l=1, m_l = 0, m_s=-1/2
n = 2, l=1, m_l = 0, m_s=+1/2
n = 2, l=1, m_l = 1, m_s=-1/2
n = 2, l=1, m_l = 1, m_s=+1/2

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Possible Quantum numbers

n = 1 l=0 m_l = 0 m_s=-1/2
m_s=+1/2

n = 2 l=0 m_l = 0 m_s=-1/2
m_s=+1/2

l=1 m_l = -1 m_s=-1/2
m_s=+1/2
m_l = 0 m_s=-1/2
m_s=+1/2
m_l = 1 m_s=-1/2
m_s=+1/2

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What do these numbers mean?

n is like the Bohr orbit number. It gives the "shell" the electron is in.

l is the orbital number, it specifies the type of orbital within the same shell.

m_l gives the orientation of the orbital – these are different flavors of the same orbital

m_s is the magnetic spin of the electron (think N and S pole) – this is specific to the electron not the orbital

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Shorthand Notation

Orbitals are specified by letters:

l=0 is an s orbital

l=1 is a p orbital

l=2 is a d orbital

l=3 is an f orbital

l=4 is a g orbital (then h, i, j, k…)

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Shorthand notation

n=1, l=0 is called a 1s orbital
n=2, l=0 is called a 2s
n=2, l=1 is called a 2p
n=3, l=2 is called a 3d

The number of electrons in each orbital are indicated as a superscript.

$1s^2$ means 2 electrons are in the 1s orbital
$3d^7$ means 7 electrons are in the 3d orbital

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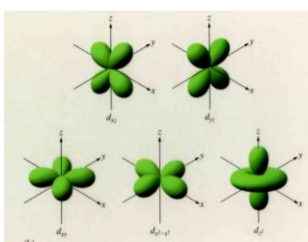
d-Orbitals



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Rules Governing Electrons

1. Pauli Exclusion Principle - No two electrons in an atom can have the same 4 quantum numbers
2. Lowest energy orbitals fill first
3. Hund's rule – Electrons pair up as a last resort
4. An orbital being full or half-full is good! (lower in energy)

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Energy of the Orbitals

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f 5g
6s 6p 6d 6f 6g 6h
7s 7p 7d 7f 7g 7h 7i

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Pauli Exclusion Principle

This determines the number of orbitals in a shell and the total number of electrons that fit in each orbit.

There is only 1 orbital (s) in the 1st shell of only 1 type which can hold, at most, 2 electrons.

There are 2 different orbitals (s, p) in the 2nd shell. There is 1 type of s (always) and 3 types of p (always). Each type can hold 2 electrons. So, at most, the 2nd shell can hold 8 electrons.

Etc.

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Electron Configurations

If you need to figure out the electron configuration, you just count the electrons and start filling from lowest energy to highest.

For example, consider C

Carbon has 6 electrons, where do they go.

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Carbon

C – 6 electrons

1s is the lowest energy orbital, it takes 2

2s is the next lowest, it also takes 2

2p comes next, it can take up to 6, so it gets the last 2 electrons

$1s^2 2s^2 2p^2$

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What’s the electron configuration of Mg?

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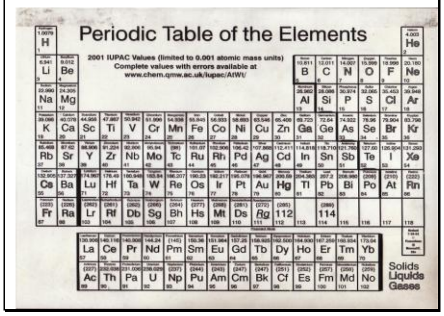

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Mg = 12 electrons

1s gets 2
2s gets 2
2p gets 6
3s gets 2

$1s^2 2s^2 2p^6 3s^2$

Slide 60

Clicker question

What is the ground state electron configuration of N?

A. $1s^2 2s^5$
B. $1s^2 2s^2 2p^3$
C. $1s^2 2s^2 2p^5$
D. $1s^2 2p^5$

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Clicker question

What is the ground state electron configuration of As?

A. $1s^22s^22p^63s^23p^83d^{10}4p^3$
B. $1s^22s^22p^63s^23p^64s^24p^3$
C. $1s^22s^22p^63s^23p^64s^23d^{10}4p^3$
D. $1s^22s^22p^63s^23p^63d^{10}4p^5$

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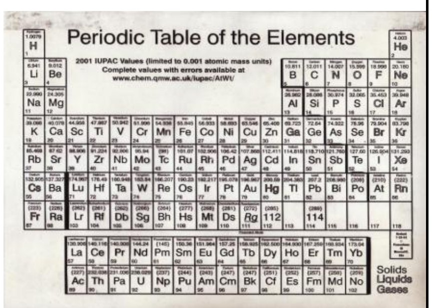

Slide 63

Clicker question

What is the ground state electron configuration of Cr?

A. $1s^22s^22p^63s^23p^83d^4$
B. $1s^22s^22p^63s^23p^64s^23d^4$
C. $1s^22s^22p^63s^23p^64s^13d^5$
D. $1s^22s^22p^63s^23p^63d^6$

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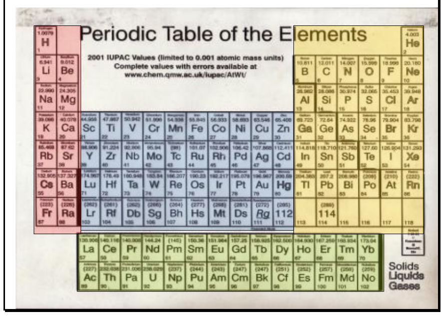

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Core vs. Valence Electrons

Core electrons – completed shells
Valence electrons – "outer" or incomplete shells

Only the valence electrons affect the chemistry of an atom.

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What's the valence configuration of…

Ca?

[Ar]4s^2

Mo?
[Kr]5s^{1}4d^5

Ga?
[Ar]4s^{2}3d^{10}4p^1 (3 valence electrons)

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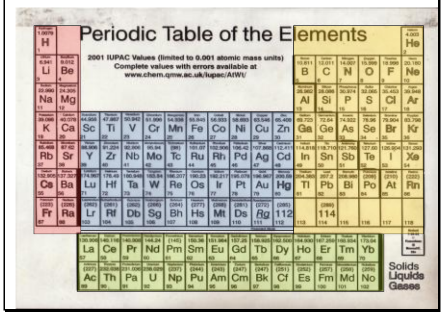

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What about Fe^{3+}?

Fe (atomic number 26)

$[Ar]4s^2 3d^6$

Take away 3 electrons…

$[Ar]4s^2 3d^3$

OR

$[Ar]3d^5$

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Power (Watts) measures the rate of energy emitted.

How many photons do you get from a 100 Watt red (700 nm) bulb in 1 second?

1 W = 1 J/s

100 J/s*1 s = 100 J

(that's why your electric bill charges you kW-hr – you pay by the joule!)

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How many photons do you get from a 100 Watt red (700 nm) bulb in 1 second?

100 J/s*1 s = 100 J total energy

$E = h * \nu = h * (c/\lambda)$

$E = 6.626 \times 10^{-34}$ Js * (3×10^{8} m/s/700×10^{-9} m)

E= 2.840×10^{-19} J/photon

100 J * $\frac{\text{1 photon}}{2.840 \times 10^{-19}\ \text{J}}$ = 3.52×10^{20} photons

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Clicker

How many 700 nm photons does it take to generate 1.00 Joules of energy?

A. 2.16×10^{48}

B. 2.16×10^{39}

C. 3.5×10^{18}

D. 2.84×10^{-19}

E. 3.5×10^{27}