Slide 1

Electronic Structure of Atoms

Chemistry is Electrons

Slide 2

What's this thing called light?

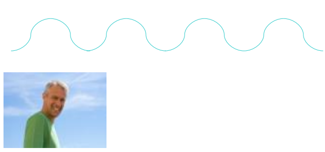
Light is an oscillating electromagnetic wave!

There are two ways to look at any wave:

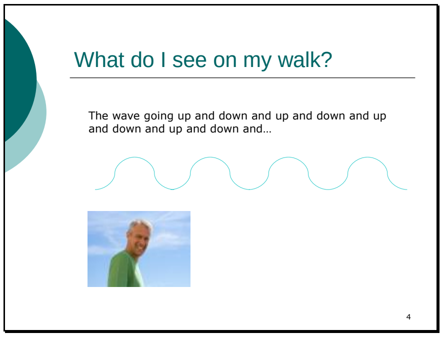
A) Freeze the wave and walk along it.
B) Stay put and watch the wave go by.

Slide 3

Freeze the wave and walk…



Slide 4



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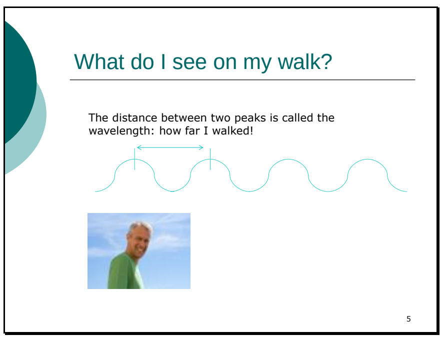

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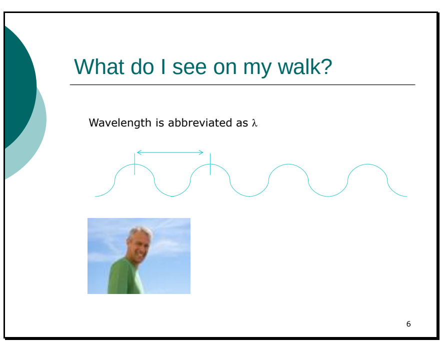
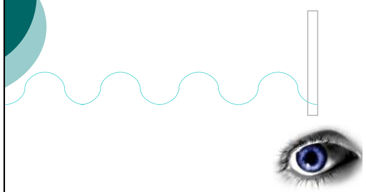


Slide 7

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



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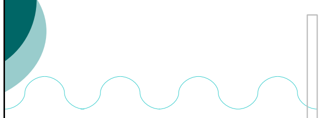
Slide 8

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")

8

Slide 9

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?
$\frac{\#}{\text{sec}}$ (or the equivalent)

9

Slide 10

What do you get when you combine distance and time?

VELOCITY!!!

Distance per Time

Miles per hour
Meters per second
Kilometers per day

10

Slide 11

$\lambda\nu=c$

Where c is the speed of light.

The speed of light is actually constant in vacuum and has a value of $2.997\text{x}10^8$ m/s or ($3.00\ \text{x}10^8$ m/s)

Why constant in vacuum?

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Slide 12

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.

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Slide 13

What is the frequency of 600 nm orange light?

c=$\lambda\nu$

$c = 3.00 \times 10^{8}\,\frac{m}{s}$ (in vacuum)

$$3.00 \times 10^{8}\,\frac{m}{s} = 600\,nm * \nu$$

UNITS! UNITS! UNITS!

$$3.00 \times 10^{8}\,\frac{m}{s} = 600\,nm * \frac{10^{-9}m}{nm} * \nu$$

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

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Slide 14

Light is another form of energy!

Important Fact #1

Light is just another form of energy.

[But it is special, behaving differently than we might expect.]

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Slide 15

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Slide 16

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!

16

Slide 17

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.

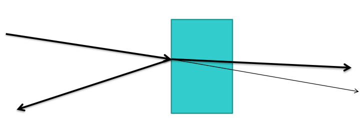
Think of the ocean and compare a tsunami to a million ripples…

17

Slide 18

When light strikes matter…

What happens? Or what COULD happen?



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Slide 19

When light strikes matter…

What happens? Or what COULD happen?

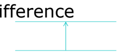
1. It bounces off.
2. It goes right through.
3. It gets absorbed.

Slide 20

Absorbed light

Important Fact #2:
Absorbing light becomes a means of probing matter.

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



Slide 21

Different wavelengths of light interact with different things:

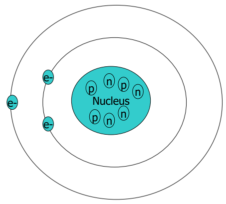
Infrared light (longer than 700 nm) interacts with the vibrations of bonds.

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

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

Slide 22

The Bohr Model and the Photoelectric effect.



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

Slide 23

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".

Slide 24

Stupid Clicker Question

I hit your rubber body with a 1000 lb truck going 50 mph and you land 1 mile away. If I hit you consecutively with two 500 lb trucks going 50 mph, do you land…

A. More than 1 mile away
B. 1 mile away
C. Less than 1 mile away
D. I'm offended by the whole idea of this question

Slide 25

You are an electron. I hit you with a 50 lb mallet and you move up two orbitals. If I hit you consecutively with 2-25lb mallets, do you:

A. Go up less than 2 orbitals
B. Go up 2 orbitals
C. Go up more than 2 orbitals
D. Stay put and throw the finger
E. Your mother

25

Slide 26

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?

26

Slide 27

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^{-19} 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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Slide 28

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).

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Slide 29

Enter Planck and his constant

$$E = h\gamma$$

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

h=Planck's constant = 6.626x10^{-34} J s

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Slide 30

How much energy does a 600 nm orange photon possess?

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

$$E = 6.626 \times 10^{-34} Js(\frac{3.00 \times 10^{8} m/s}{600 \times 10^{-9} m})$$

E= 3.313x10^{-19} J in a single photon

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Slide 31

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:

$4 * 3.313 \times 10^{-19}$ J = 1.33×10^{-18} J

That should be enough to knock my electron off!

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Slide 32

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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Slide 33

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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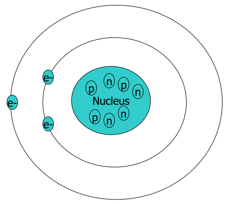
Slide 34

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



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Slide 35

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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Slide 36

Chemical Reactivity…

…is all about the electrons.

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Slide 37

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

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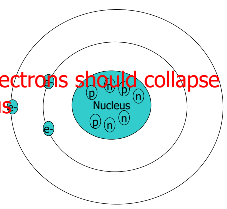
Slide 38

What's wrong with the Bohr Model?



The electrons should collapse into the nucleus

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Slide 39

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).

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Slide 40

It's CSI!

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

The energy of the transition is just:

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

The math gets complicated in a hurry…

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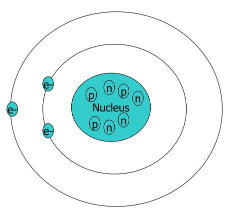
Slide 41

It's just charge to charge attraction…



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

41

Slide 42

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.

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

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Important Facts about Light and Matter

1. Important Fact #1 – Light is just another form of energy
2. Important Fact #2 – For light to be absorbed, it must be tuned to a specific energy transition in matter.

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Slide 44

Quantum electronic structure

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

Important Fact #3

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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Important Chapter 7 Fact #4

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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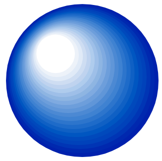
Electron Orbitals



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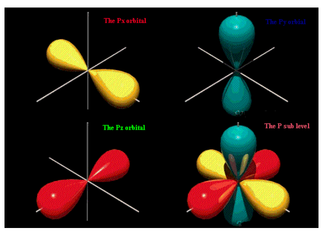
p-orbital



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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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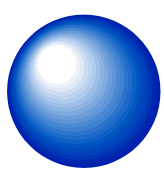
s-orbital   (l=0)



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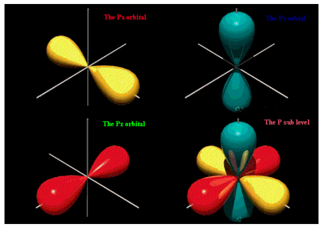
p-orbital (l=1)



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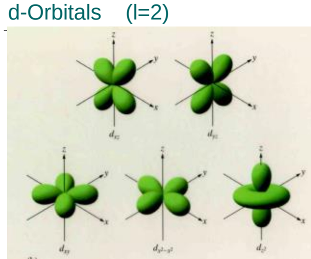
d-Orbitals (l=2)



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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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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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Pauli Exclusion Principle

Every electron has a unique address.

n=principal quantum number
n=# of different types of orbitals

n=1 – only 1 type (s)
n=2 – 2 types (s, p)
n=3 – 3 types (s, p, d

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m_l = # of orientations
m_l = -l, -l+1, …0…1, 2…l
m_l = 2l+1

l=0, m_l = 2(0) + 1 = 1
l=1, m_l = 2(1) + 1 = 3
l=2, m_l = 2(2) + 1 = 5
etc.

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m_s = +1/2, -1/2

So you can put 2 electrons in each orbital!

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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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So, take a principal quantum number like n=4

n=4 will have 4 orbital types (s, p, d, f)

Based on the l values, there is 1 s orbital (2(0)+1), 3 p orbitals (2(1) +1), 5 d orbitals and 7 f orbitals.

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Slide 64

Based on the l values, there is 1 s orbital (2(0)+1), 3 p orbitals (2(1) +1), 5 d orbitals and 7 f orbitals.

So that is a total of 16 orbitals (1+3+5+7). Each orbital can hold 2 electrons, so you can get 32 electrons in your n=4 orbit.

The other way to see that is:
1 s orbital – 2 electrons
3 p orbitals – 6 electrons
5 d orbitals – 10 electrons
7 f orbitals – 14 electrons

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If n=7…how many different shape orbitals are there?

A. 5
B. 7
C. 14
D. 30
E. 64

Slide 66

How many electrons could you put in n=7?

A.32
B.64
C 98
D. 216
E 70

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Rules Governing Electrons

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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

So, 1s fills first then 2s, then 2p, then 3s then 3p then 4s!!!

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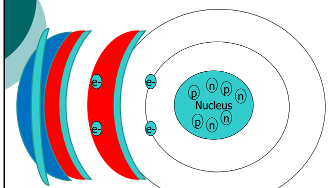
It's just charge to charge attraction…



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

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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

Notice that the next s always fills before the d (5s before 4d, 6s before 5d)

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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

And look at the f's!

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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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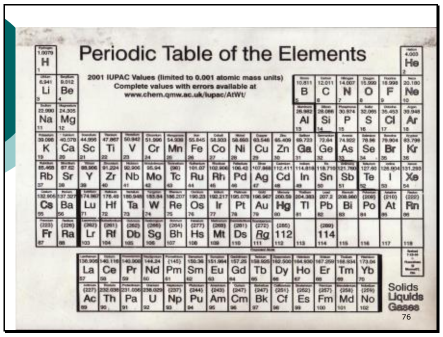

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Mg = 12 electrons

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

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

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Slide 78

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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Slide 79

Clicker question

What is the ground state electron configuration of As?

A. $1s^2 2s^2 2p^6 3s^2 3p^8 3d^{10} 4p^3$
B. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 4p^3$
C. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$
D. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4p^5$
E. I love you

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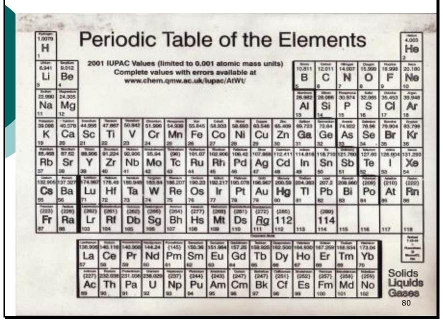

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Clicker question

What is the ground state electron configuration of Cr?

A. $1s^2 2s^2 2p^6 3s^2 3p^8 3d^4$
B. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^4$
C. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$
D. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$

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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) – d orbitals

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....$4s^2 3d^9$

...$4s^1 3d^{10}$

83

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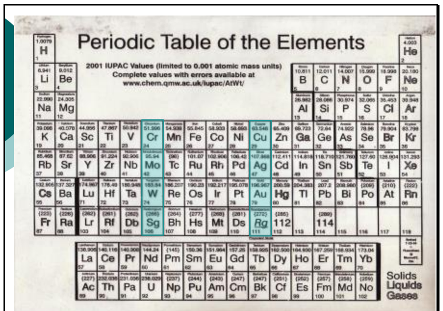
Slide 84



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If you are s^2d^4 you are more stable as s^1d^5

If you are s^2d^9 you are more stable as s^1d^{10}

[Note: If you look at the actual configurations as printed on some periodic tables, you'll notice other exceptions. I'm not holding you responsible for those.]

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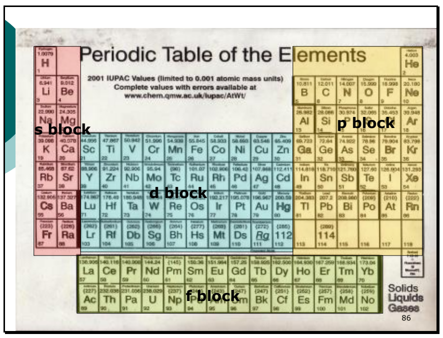

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Core vs. Valence Electrons

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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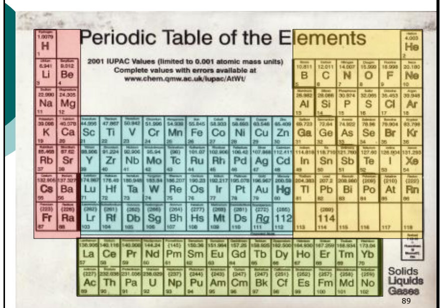

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What about Fe^{3+}?

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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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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Electron pairing affects magnetism

It is not apparent in the simple electron configuration.

Consider C again. Its configuration is $1s^2 2s^2 2p^2$

Since the 1s and 2s orbitals are full there's no choice with the electrons, but the 2p is mostly empty.

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Electron configurations

Another way to show the electron configurations is to actually show each orbital.

Electrons are represented by arrows pointing up (m_s = +1/2) or down (m_s = -1/2)

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Carbon – 2 possibilities

↑↓ ↑↓ ↑ ↑ ___

1s 2s 2p

↑↓ ↑↓ ↑↓ ___ ___

1s 2s 2p

This is where Hund's rule comes into play.

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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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Carbon – only 1 possibility

↑↓ ↑↓ ↑ ↑ ___

1s 2s 2p

~~↑↓ ↑↓ ↑↓ ___ ___~~

~~1s 2s 2p~~

Hund's rule – Electrons pair up as a last resort

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What difference does it make?

I'm glad you asked!

Paramagnetism – Only atoms with unpaired electrons are attracted to magnetic fields.

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Carbon – 2 possibilities

1s	2s	2p		
↑↓	↑↓	↑	↑	

Paramagnetic

1s	2s	2p		
↑↓	↑↓	↑↓		

Not paramagnetic

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Photons as a source of energy

Did anyone own an Easy Bake oven?

Cooking with a light bulb!

It's just another source of energy…but it must be absorbed!

Heat energy is automatically shared from colliding molecules. Light energy must be absorbed by the

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Slide 100

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 * ν = h * (c/λ)

$$E = \frac{hc}{\lambda} = \frac{(6.626x10^{-34}Js)3x10^{8}\frac{m}{s}}{700x10^{-9}m}$$

E= $2.840x10^{-19}$ J/photon

100 J * $\frac{1 \text{ photon}}{2.840x10^{-19} \text{ J}}$ = $3.52x10^{20}$ photons

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Clicker

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

A. $2.16x10^{48}$

B. $2.16x10^{39}$

C. $3.5x10^{18}$

D. $2.84x10^{-19}$

E. $3.5x10^{27}$

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From earlier 700 nm corresponds to 2.84×10^{-19} J/photon

$$1.00\,J\;\frac{1\;photon}{2.84\times10^{-19}J} = 3.52\times10^{18}\;photons$$

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A little problem

I want to heat 100 g of water from 25ºC to the normal boiling point. How much energy do I need to add to the water?

A. 31.3 J
B. 31,350 J
C. 10, 450 J
D. None of the above
E. I don't know, but I love this class.

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$$q = mc\Delta T$$

$$q = 100\;g\left(4.18\;\frac{J}{g℃}\right)(100℃ - 25℃)$$

$$q = 31{,}350\;J$$

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How many 700 nm photons would I need to absorb to heat my water?

A. 4.6×10^{-40} photons
B. 1.1×10^{14} photons
C. 1.1×10^{23} photons
D. 8.9×10^{-15} photons
E. 4.6×10^{-49} photons

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$$31{,}350\,J \frac{1\,photon}{2.84 \times 10^{-19} J} = 1.1 \times 10^{23} photons$$

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Slide 108

Suppose I have a 100 W red (700 nm) light bulb. How long would it take to heat my water if the water is absorbing 35% of the light emitted by the bulb? [Assuming it all stays in the water.]

A. 1100 s
B. 1.1×10^{6} s
C. 896 s
D. 89 s
E. All frigging day

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35% absorbed $= \frac{35\ photons\ absorbed}{100\ photons\ incident}$

$$= \frac{35\ J\ absorbed}{100\ J\ incident}$$

$$100\ W = \frac{100\ J}{s}$$

$$31350\ J\ absorbed \frac{100\ J\ inc}{35\ J\ absorbed} \frac{1\ s}{100\ J\ incident} = 896\ s$$