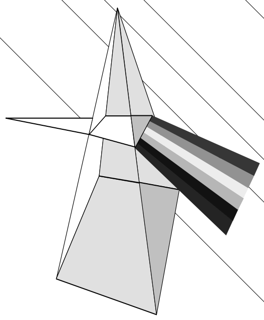


Chapter 7

Atomic Structure

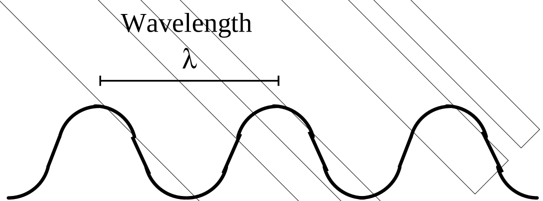
1

Light

- **Made up of electromagnetic radiation**
- **Waves of electric and magnetic fields at right angles to each other.**

2

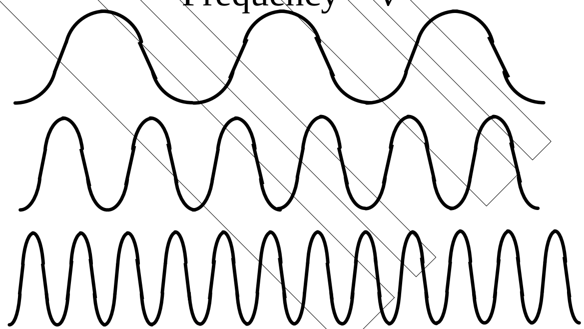
Parts of a wave



Frequency = number of cycles in one second
Measured in hertz 1 hertz = 1 cycle/second

3

Frequency = ν



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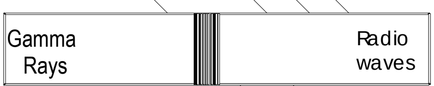
Kinds of EM waves

- **There are many**
- **different λ and ν**
- **Radio waves, microwaves, x rays and gamma rays are all examples**
- **Light is only the part our eyes can detect**



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The speed of light

- **in a vacuum is 2.998×10^8 m/s**
- **= c**
- **$c = \lambda\nu$**
- **What is the wavelength of light with a frequency 5.89×10^5 Hz?**
- **What is the frequency of blue light with a wavelength of 484 nm?**

6

In 1900

- Matter and energy were seen as different from each other in fundamental ways
- Matter was particles
- Energy could come in waves, with any frequency.
- Max Planck found that the cooling of hot objects couldn't be explained by viewing energy as a wave.

7

Energy is Quantized

- Planck found ΔE came in chunks with size $h\nu$
- $\Delta E = nh\nu$
- where n is an integer.
- and h is Planck's constant
- $h = 6.626 \times 10^{-34}$ J s
- these packets of $h\nu$ are called quantum

8

Einstein is next

- Said electromagnetic radiation is quantized in particles called photons
- Each photon has energy = $h\nu = hc/\lambda$
- Combine this with $E = mc^2$
- you get the apparent mass of a photon
- $m = h / (\lambda c)$

9

Which is it?

- Is energy a wave like light, or a particle?
- Yes
- Concept is called the Wave -Particle duality.
- What about the other way, is matter a wave?
- Yes

10

Matter as a wave

- Using the velocity v instead of the frequency ν we get
- De Broglie's equation $\lambda = h/mv$
- can calculate the wavelength of an object

11

Examples

- The laser light of a CD is 7.80×10^2 m. What is the frequency of this light?
- What is the energy of a photon of this light?
- What is the apparent mass of a photon of this light?
- What is the energy of a mole of these photons?

12

What is the wavelength?

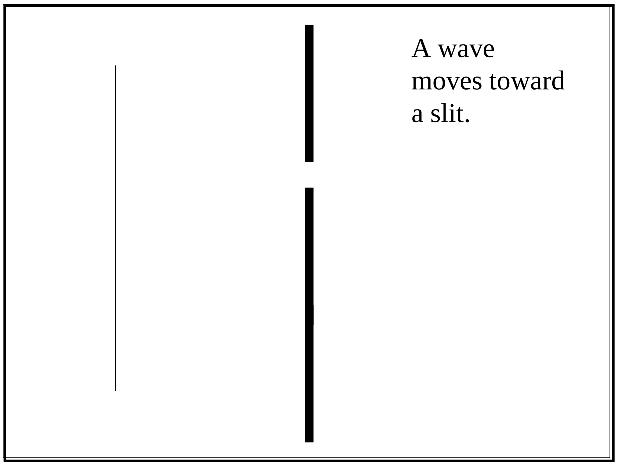
- **of an electron with a mass of 9.11×10^{-31} kg traveling at 1.0×10^{7} m/s?**
- **Of a softball with a mass of 0.10 kg moving at 125 mi/hr?**

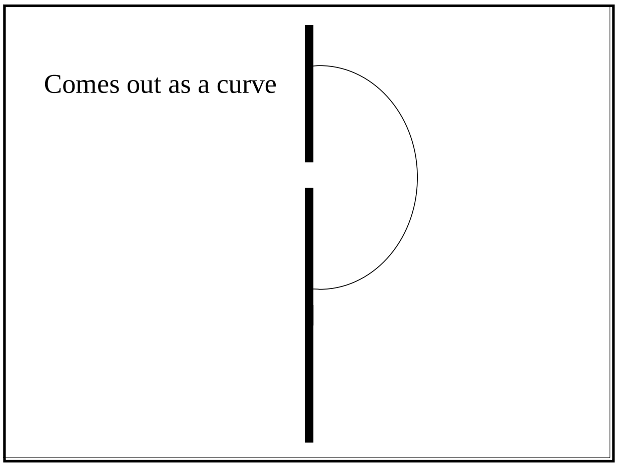
13

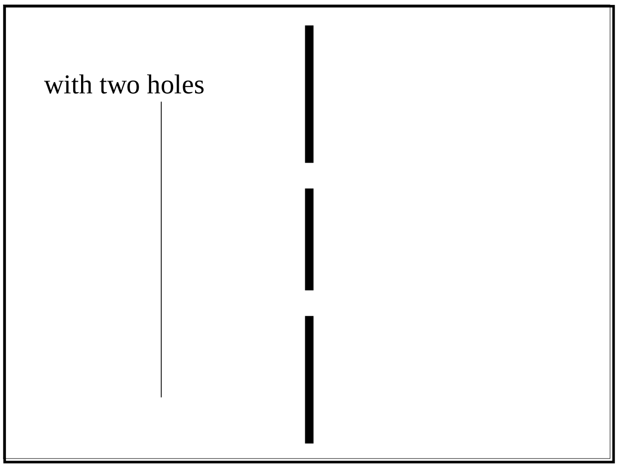
How do they know?

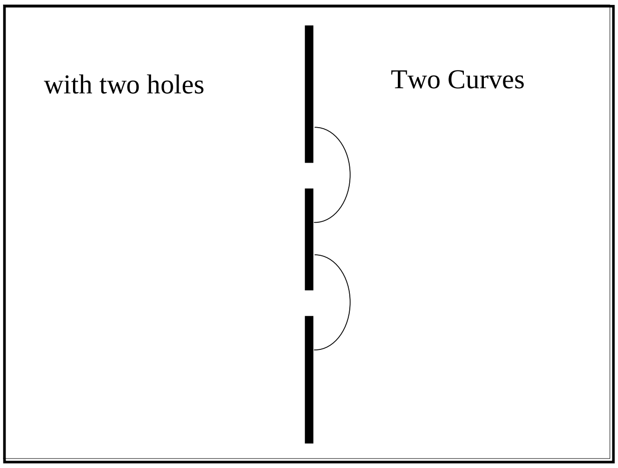
- **When light passes through, or reflects off, a series of thinly spaced lines, it creates a rainbow effect**
- **because the waves interfere with each other.**

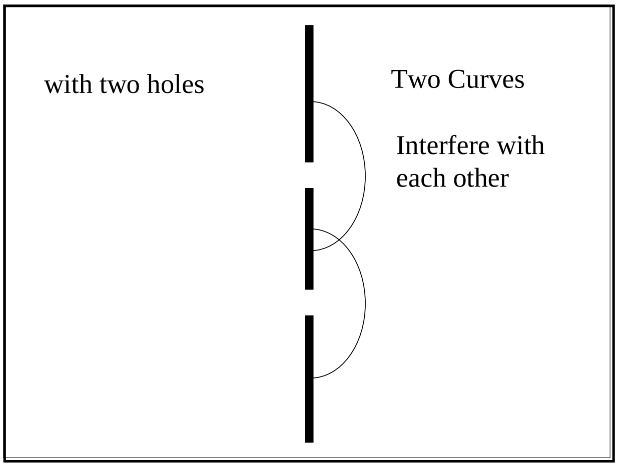
14

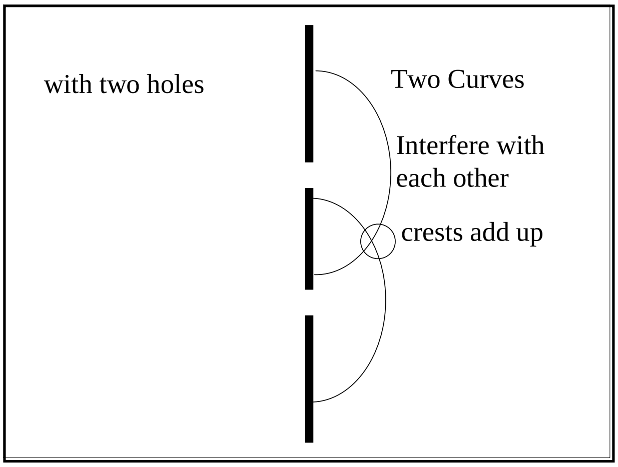


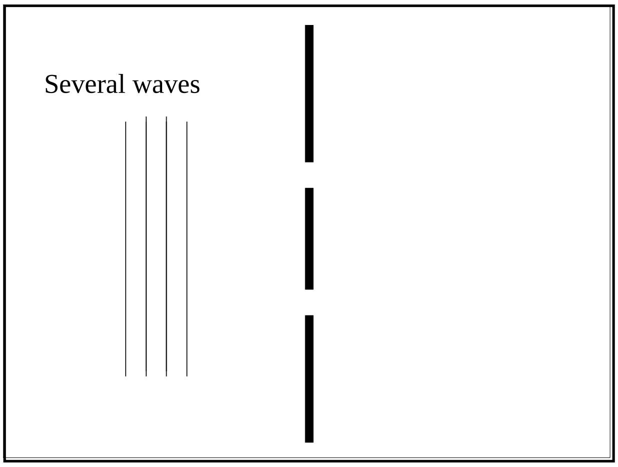


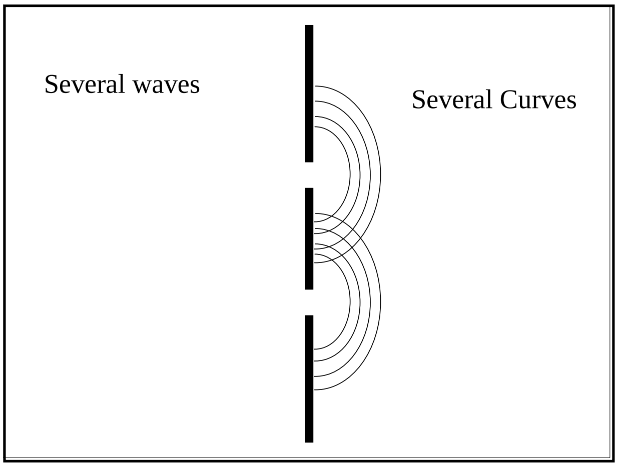


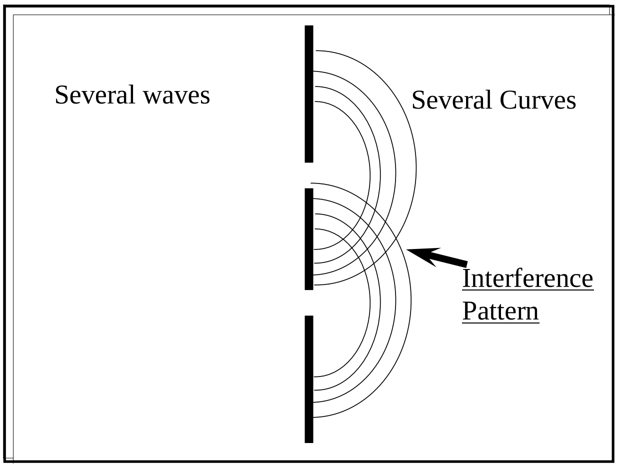










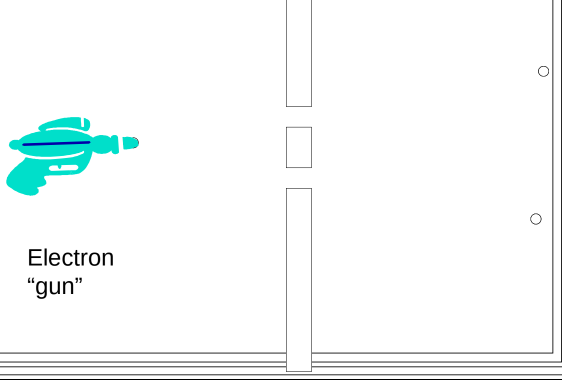


What will an electron do?

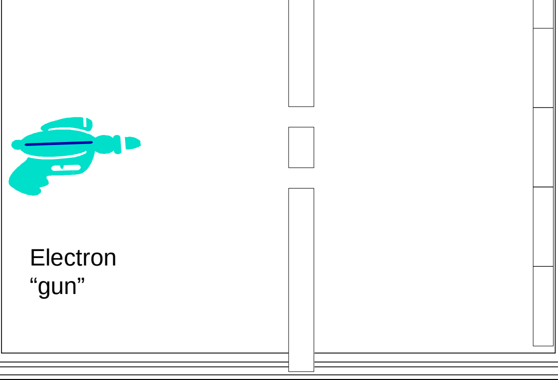
- **It has mass, so it is matter.**
- **A particle can only go through one hole**
- **A wave goes through both holes**
- **Light shows <u>interference patterns</u>**

24

Electron as Particle



Electron as wave



Which did it do?

- It made the diffraction pattern
- The electron is a wave
- Led to Schrödingers equation

What will an electron do?

- **An electron does go though both, and makes an interference pattern.**
- **It behaves like a wave.**
- **Other matter has wavelengths too short to notice.**

Image

28

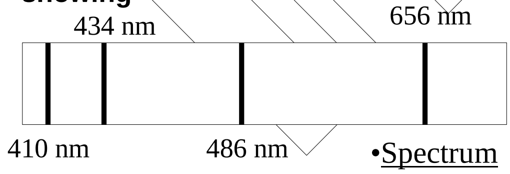
Spectrum

- **The range of frequencies present in light.**
- **White light has a continuous spectrum.**
- **All the colors are possible.**
- **A rainbow.**

29

Hydrogen spectrum

- **Emission spectrum because these are the colors it gives off or emits**
- **Called a line spectrum.**
- **There are just a few discrete lines showing**



•Spectrum

30

What this means

- Only certain energies are allowed for the hydrogen atom.
- Can only give off certain energies.
- Use ΔE = hν = hc / λ
- Energy in the atom is quantized

31

Niels Bohr

- Developed the quantum model of the hydrogen atom.
- He said the atom was like a solar system
- The electrons were attracted to the nucleus because of opposite charges.
- Didn't fall in to the nucleus because it was moving around

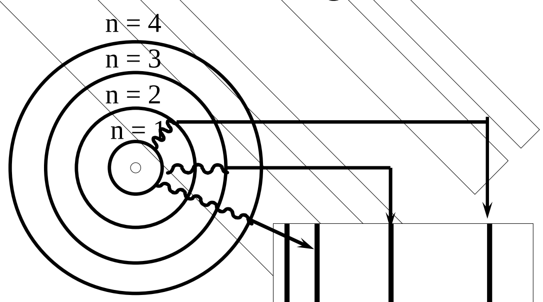
32

The Bohr Ring Atom

- He didn't know why but only certain energies were allowed.
- He called these allowed energies energy levels.
- Putting energy into the atom moved the electron away from the nucleus
- From ground state to excited state.
- When it returns to ground state it gives off light of a certain energy

33

The Bohr Ring Atom



34

The Bohr Model

- n is the energy level
- for each energy level the energy is
- Z is the nuclear charge, which is +1 for hydrogen.
- $E = -2.178 \times 10^{-18}$ J (Z^2 / n^2)
- n = 1 is called the ground state
- when the electron is removed, n = ∞
- E = 0

35

We are worried about the change

- When the electron moves from one energy level to another.
- $\Delta E = E_{final} - E_{initial}$
- $\Delta E = -2.178 \times 10^{-18}$ J $Z^2 (1/ n_f^2 - 1/ n_i^2)$

36

Examples

- Calculate the energy need to move an electron from its to the third energy level.
- Calculate the energy released when an electron moves from n= 4 to n=2 in a hydrogen atom.
- Calculate the energy released when an electron moves from n= 5 to n=3 in a He^{+1} ion

37

When is it true?

- Only for hydrogen atoms and other monoelectronic species.
- Why the negative sign?
- To increase the energy of the electron you make it further to the nucleus.
- the maximum energy an electron can have is zero, at an infinite distance.

38

The Bohr Model

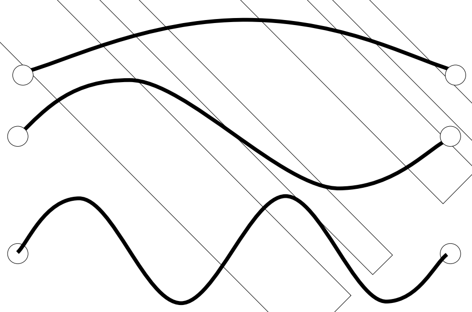
- Doesn't work
- only works for hydrogen atoms
- electrons don't move in circles
- the quantization of energy is right, but not because they are circling like planets.

39

The Quantum Mechanical Model

- A totally new approach
- De Broglie said matter could be like a wave.
- De Broglie said they were like standing waves.
- The vibrations of a stringed instrument

40



41

What's possible?

- You can only have a standing wave if you have complete waves.
- There are only certain allowed waves.
- In the atom there are certain allowed waves called electrons.
- 1925 Erwin Schroedinger described the wave function of the electron
- Much math, but what is important are the solutions

42

Schrödinger's Equation

- The wave function is a F(x, y, z)
- Actually F(r,θ,φ)
- Solutions to the equation are called orbitals.
- These are not Bohr orbits.
- Each solution is tied to a certain energy
- These are the energy levels

•**Animation**

43

There is a limit to what we can know

- We can't know how the electron is moving or how it gets from one energy level to another.
- The Heisenberg Uncertainty Principle
- There is a limit to how well we can know both the position and the momentum of an object.

44

Mathematically

- $\Delta x \cdot \Delta(mv) > h/4\pi$
- Δx is the uncertainty in the position
- $\Delta(mv)$ is the uncertainty in the momentum.
- the minimum uncertainty is $h/4\pi$

45

Examples

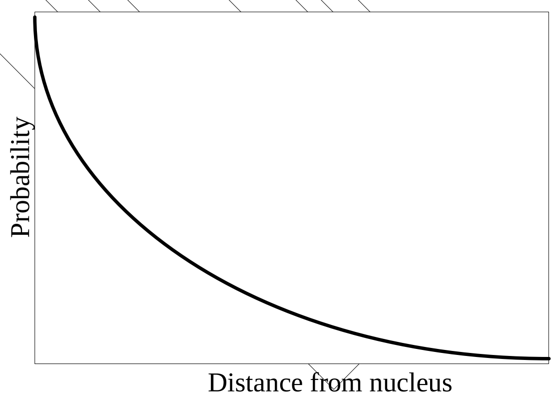
- What is the uncertainty in the position of an electron. mass 9.31×10^{-31} kg with an uncertainty in the speed of 0.100 m/s
- What is the uncertainty in the position of a baseball, mass 0.145 kg with an uncertainty in the speed of 0.100 m/s

46

What does the wave Function mean?

- nothing.
- it is not possible to visually map it.
- The square of the function is the probability of finding an electron near a particular spot.
- best way to visualize it is by mapping the places where the electron is likely to be found.

47



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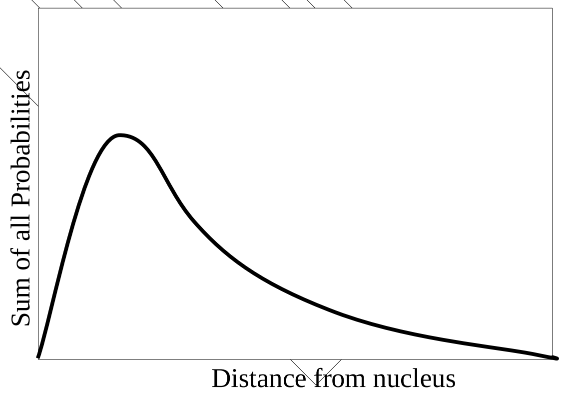


49

Defining the size

- The nodal surface.
- The size that encloses 90% to the total electron probability.
- NOT at a certain distance, but a most likely distance.
- For the first solution it is a a sphere.

50

Quantum Numbers

- There are many solutions to Schrödinger's equation
- Each solution can be described with quantum numbers that describe some aspect of the solution.
- Principal quantum number (n) size and energy of an orbital
- Has integer values >0

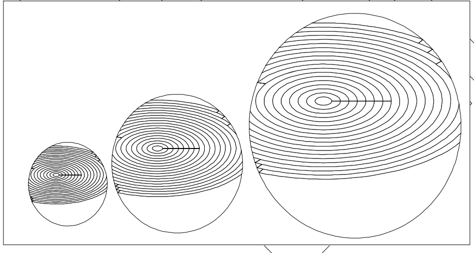
51

Quantum numbers

- Angular momentum quantum number l
- shape of the orbital
- integer values from 0 to n-1
- l = 0 is called s
- l = 1 is called p
- l =2 is called d
- l =3 is called f
- l =4 is called g

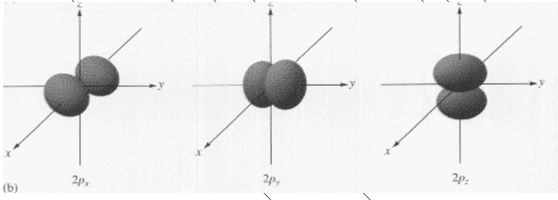
52

S orbitals



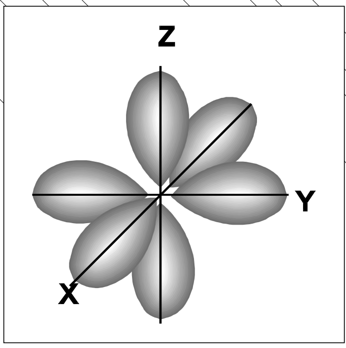
53

P orbitals



54

P Orbitals



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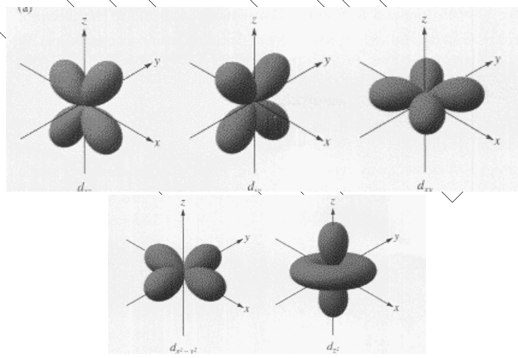
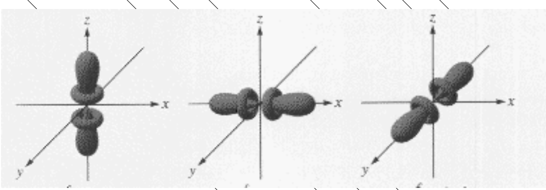
D orbitals



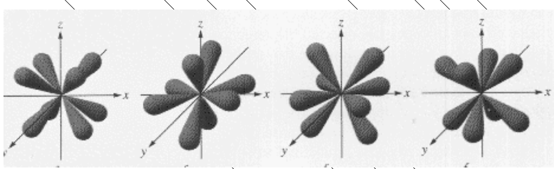
56

F orbitals



57

F orbitals



58

Quantum numbers

- **Magnetic quantum number (m_l)**
  - **integer values between - l and + l**
  - **tells direction in each shape**
- **Electron spin quantum number (m_s)**
  - **Can have 2 values**
  - **either +1/2 or -1/2**

59

1. A
2. B
3. C
4. A
5. B
6. A
7. B
8. A
9. A

60

Polyelectronic Atoms

- More than one electron
- three energy contributions
- The kinetic energy of moving electrons
- The potential energy of the attraction between the nucleus and the electrons.
- The potential energy from repulsion of electrons

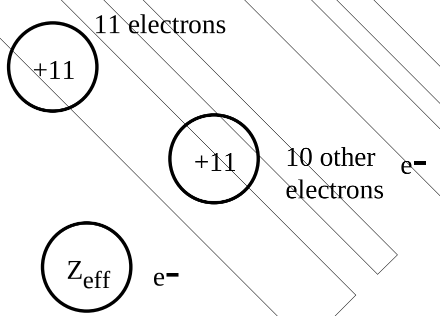
61

Polyelectronic atoms

- Can't solve Schrödinger's equation exactly
- Difficulty is repulsion of other electrons.
- Solution is to treat each electron as if it were effected by the net field of charge from the attraction of the nucleus and the repulsion of the electrons.
- Effective nuclear charge

62

Sodium Atom



63

Effective Nuclear charge

- Can be calculated from
  $E = -2.178 \times 10^{-18}\ J\ (Z_{eff}^2 / n^2)$
- and
- $\Delta E = -2.178 \times 10^{-18}\ J\ Z_{eff}^2\ (1/n_f^2 - 1/n_i^2)$

64

The Periodic Table

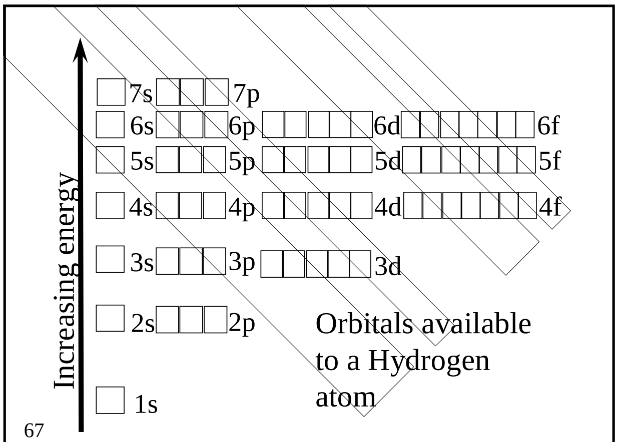
- Developed independently by German Julius Lothar Meyer and Russian Dmitri Mendeleev (1870"s)
- Didn't know much about atom.
- Put in columns by similar properties.
- Predicted properties of missing elements.

65

Aufbau Principle

- Aufbau is German for building up
- As the protons are added one by one, the electrons fill up hydrogen-like orbitals.
- Fill up in order of energy

66



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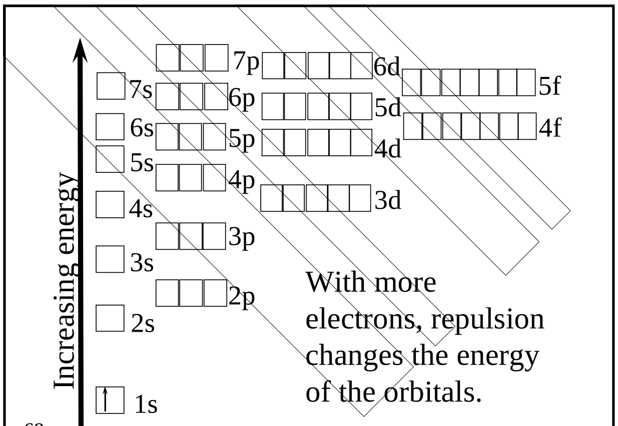

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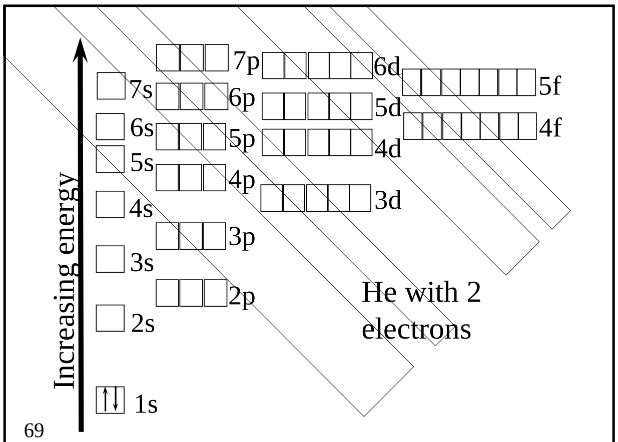

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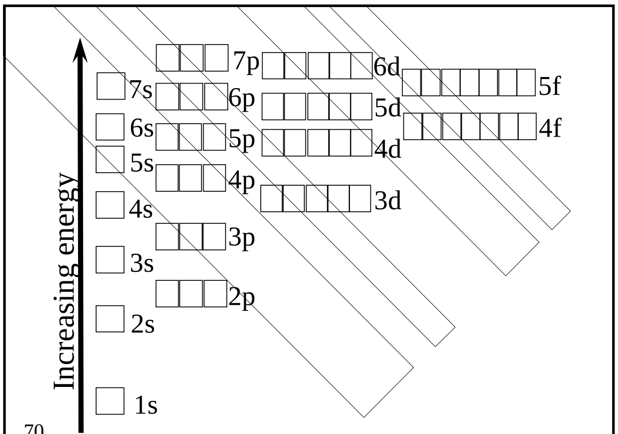


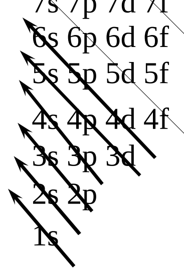
70

Details

- **Valence electrons- the electrons in the outermost energy levels (not d).**
- **Core electrons- the inner electrons**
- **Hund's Rule- The lowest energy configuration for an atom is the one have the maximum number of unpaired electrons in the orbital.**
- **C $1s^2$ $2s^2$ $2p^2$** ↑↓ ↑↓ ↑ ↑

71

Fill from the bottom up following the arrows



- $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $4s^2$ $3d^{10}$ $4p^6$ $5s^2$ $4d^{10}$ $5p^6$ $6s^2$
- [illegible] electrons

72

Details

- Elements in the same column have the same electron configuration.
- Put in columns because of similar properties.
- Similar properties because of electron configuration.
- Noble gases have filled energy levels.
- Transition metals are filling the d orbitals

73

The Shorthand

- Write the symbol of the noble gas before the element
- Then the rest of the electrons.
- Aluminum - full configuration
- $1s^2 2s^2 2p^6 3s^2 3p^1$
- Ne is $1s^2 2s^2 2p^6$
- so Al is [Ne] $3s^2 3p^1$

74

The Shorthand

Sn- 50 electrons

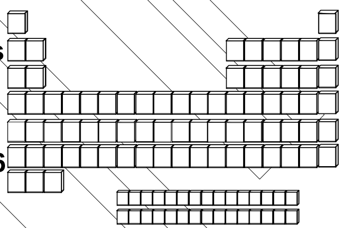
The noble gas before it is Kr

Takes care of 36

Next $5s^2$

Then $4d^{10}$

Finally $5p^2$



[Kr] $5s^2 4d^{10} 5p^2$

[Kr] $4d^{10} 5s^2 5p^2$

75

Exceptions

- Ti = [Ar] $4s^2 3d^2$
- V = [Ar] $4s^2 3d^3$
- Cr = [Ar] $4s^1 3d^5$
- Mn = [Ar] $4s^2 3d^5$
- Half filled orbitals
- Scientists aren’t certain why it happens
- same for Cu [Ar] $3d^{10} 4s^1$

76

More exceptions

- Lanthanum La: [Xe] $5d^1 6s^2$
- Cerium Ce: [Xe] $5d^1 4f^1 6s^2$
- Promethium Pr: [Xe] $4f^3 6s^2$
- Gadolinium Gd: [Xe] $4f^7 5d^1 6s^2$
- Lutetium Pr: [Xe] $4f^{14} 5d^1 6s^2$
- We’ll just pretend that all except Cu and Cr follow the rules.

77

More Polyelectronic

- We can use Z_{eff} to predict properties, if we determine it’s pattern on the periodic table.
- Can use the amount of energy it takes to remove an electron for this.
- Ionization Energy- The energy necessary to remove an electron from a gaseous atom.

78

Remember this

- $E = -2.18 \times 10^{-18}$ J(Z^2/n^2)
- was true for Bohr atom.
- Can be derived from quantum mechanical model as well
- for a mole of electrons being removed
- $E = (6.02 \times 10^{23}/\text{mol})2.18 \times 10^{-18}$ J(Z^2/n^2)
- $E = 1.13 \times 10^6$ J/mol(Z^2/n^2)
- $E = 1310$ kJ/mol(Z^2/n^2)

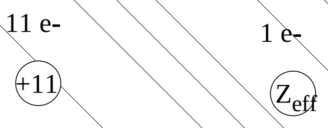
79

Example

- Calculate the ionization energy of B^{+4}

80

Remember our simplified atom



81

This gives us

- Ionization energy = 1310 kJ/mol(Z_{eff}^2/n^2)
- So we can measure Z_{eff}
- The ionization energy for a 1s electron from sodium is 1.39×10^5 kJ/mol .
- The ionization energy for a 3s electron from sodium is 4.95×10^2 kJ/mol .
- Demonstrates shielding

82

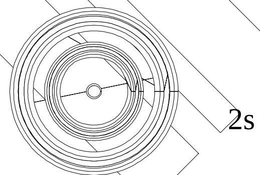
Shielding

- Electrons on the higher energy levels tend to be farther out.
- Have to look through the other electrons to see the nucleus.
- They are less effected by the nucleus.
- lower effective nuclear charge
- If shielding were completely effective, $Z_{eff} = 1$
- Why isn't it?

83

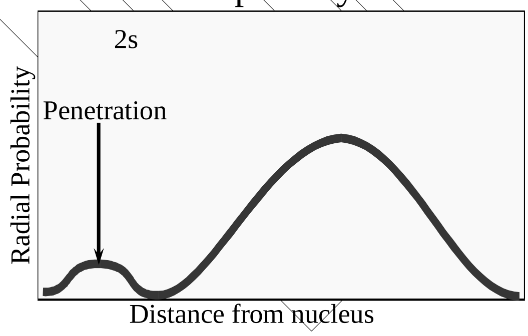
Penetration

- There are levels to the electron distribution for each orbital



84

Graphically



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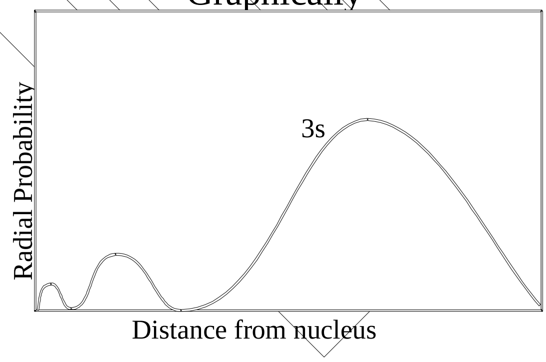
Graphically



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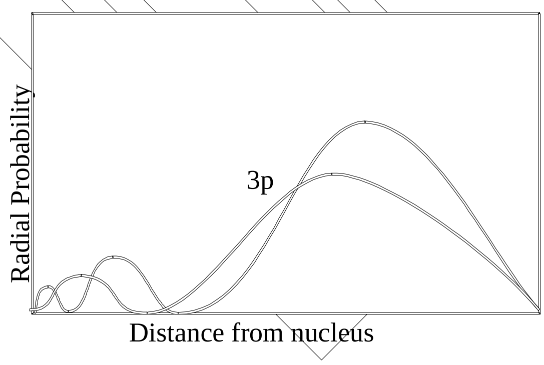

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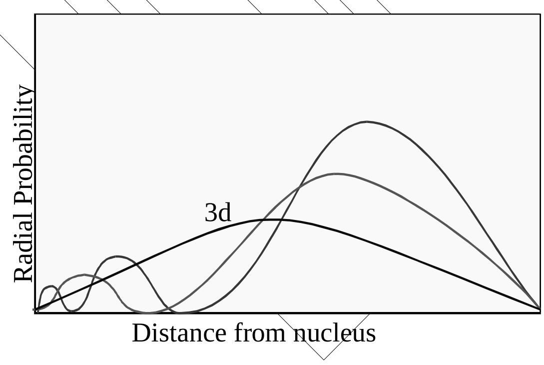

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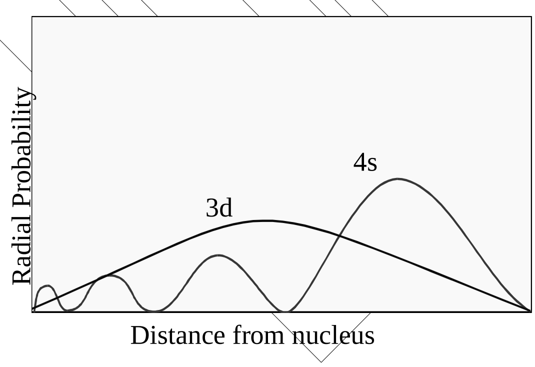


89

Penetration effect

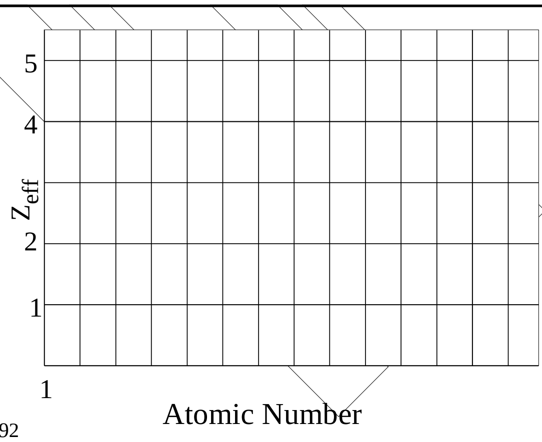
- **The outer energy levels penetrate the inner levels so the shielding of the core electrons is not totally effective.**
- **from most penetration to least penetration the order is**
- **ns > np > nd > nf (within the same energy level)**
- **This is what gives us our order of filling, electrons prefer s and p**

90

How orbitals differ

- The more positive the nucleus, the smaller the orbital.
- A sodium 1s orbital is the same shape as a hydrogen 1s orbital, but it is smaller because the electron is more strongly attracted to the nucleus.
- The helium 1s is smaller as well
- This provides for better shielding

91



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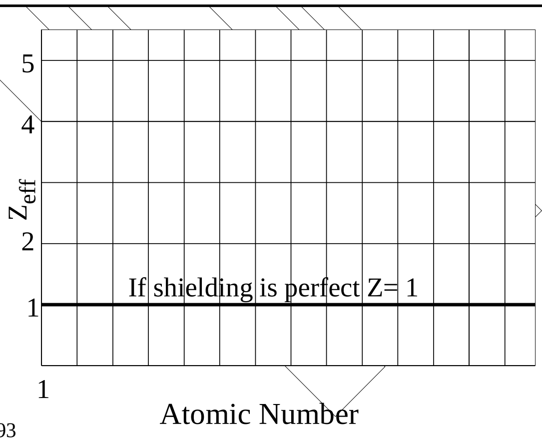

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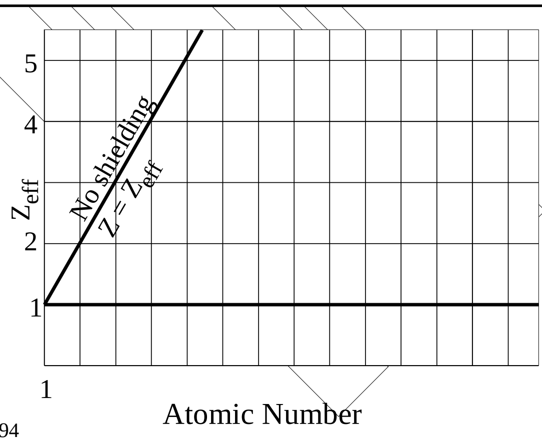

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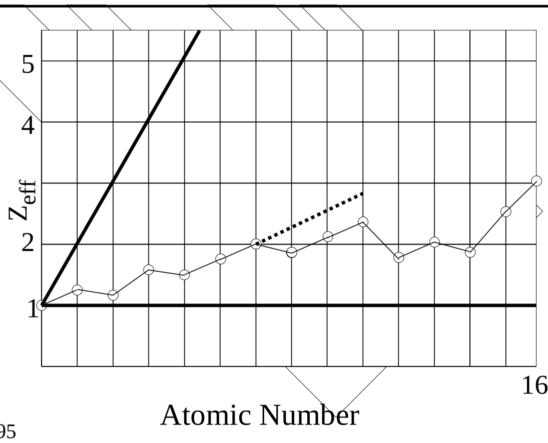


95

Periodic Trends

- Ionization energy the energy required to remove an electron form a gaseous atom
- Highest energy electron removed first.
- First ionization energy (I_1) is that required to remove the first electron.
- Second ionization energy (I_2) - the second electron
- etc. etc.

96

Trends in ionization energy

- for Mg
  - I_1 = 735 kJ/mole
  - I_2 = 1445 kJ/mole
  - I_3 = 7730 kJ/mole
- The effective nuclear charge increases as you remove electrons.
- It takes much more energy to remove a core electron than a valence electron because there is less shielding

97

Explain this trend

- For Al
  - I_1 = 580 kJ/mole
  - I_2 = 1815 kJ/mole
  - I_3 = 2740 kJ/mole
  - I_4 = 11,600 kJ/mole

98

Across a Period

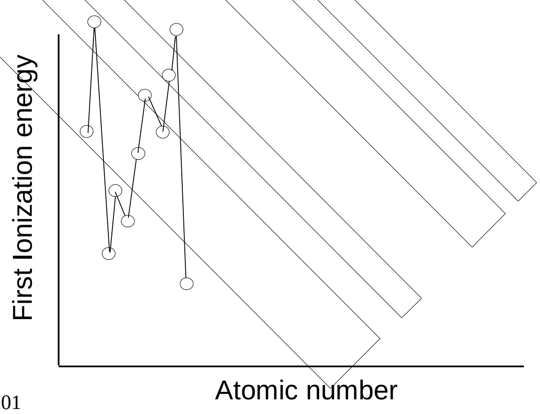
- Generally from left to right, I_1 increases because
- there is a greater nuclear charge with the same shielding.
- As you go down a group I_1 decreases because electrons are further away and there is more shielding

99

It is not that simple

- Z_{eff} changes as you go across a period, so will I_1
- Half-filled and filled orbitals are harder to remove electrons from
- here's what it looks like

100



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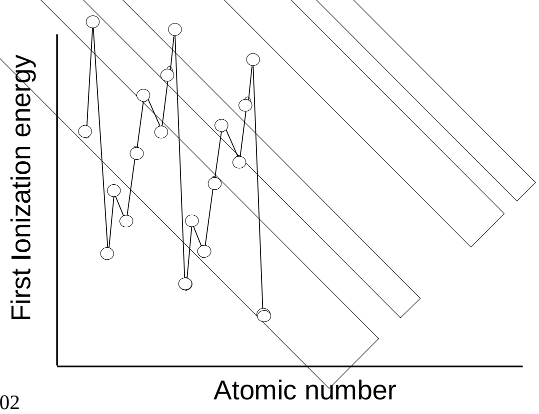

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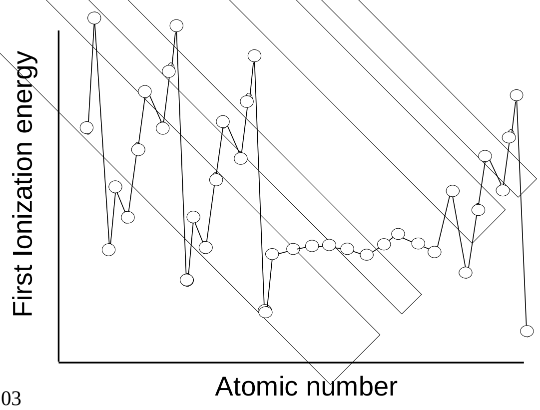


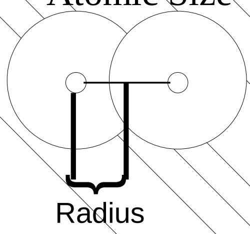
103

Atomic Size

- First problem where do you start measuring
- The electron cloud doesn't have a definite edge.
- They get around this by measuring more than 1 atom at a time

104

Atomic Size



- **Atomic Radius = half the distance between two nuclei of a diatomic molecule**

105

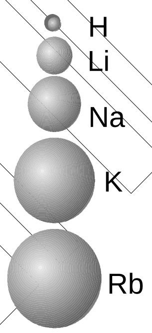
Trends in Atomic Size

- **Influenced by two factors**
- **Shielding**
- **More shielding is further away**
- **Charge on nucleus**
- **More charge pulls electrons in closer**

106

Group trends

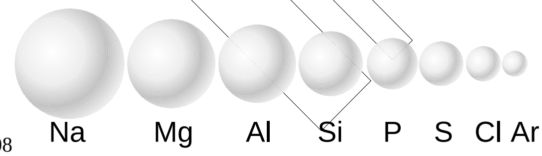
- **As we go down a group**
- **Each atom has another energy level**
- **So the atoms get bigger**



107

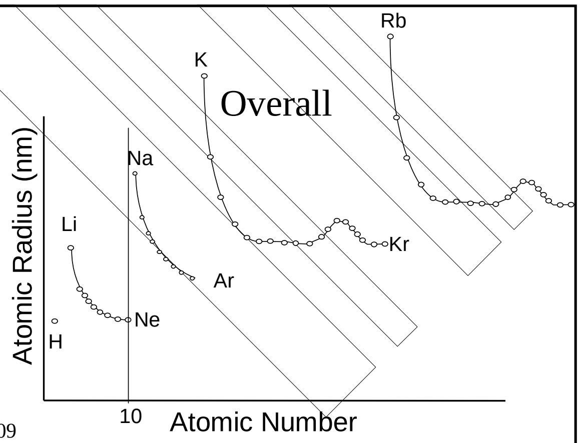
Periodic Trends

- **As you go across a period the radius gets smaller.**
- **Same energy level**
- **More nuclear charge**
- **Outermost electrons are closer**



108

Overall



109

Electron Affinity

- The energy change associated with adding an electron to a gaseous atom
- High electron affinity gives you energy-
- exothermic
- More negative
- Increase (more -) from left to right
  - greater nuclear charge.
- Decrease as we go down a group
  - More shielding

110

Ionic Size

- Cations form by losing electrons
- Cations are smaller than the atom they come from
- Metals form cations
- Cations of representative elements have noble gas configuration.

111

Ionic size

- Anions form by gaining electrons
- Anions are bigger than the atom they come from
- Nonmetals form anions
- Anions of representative elements have noble gas configuration.

112

Configuration of Ions

- Ions always have noble gas configuration
- Na is $1s^2 2s^2 2p^6 3s^1$
- Forms a 1+ ion - $1s^2 2s^2 2p^6$
- Same configuration as neon
- Metals form ions with the configuration of the noble gas before them - they lose electrons

113

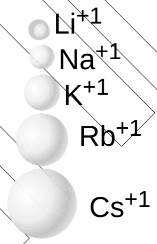
Configuration of Ions

- Non-metals form ions by gaining electrons to achieve noble gas configuration.
- They end up with the configuration of the noble gas after them.

114

Group trends

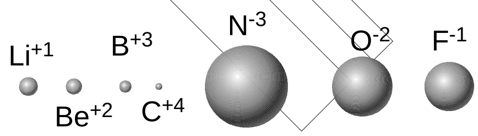
- Adding energy level
- Ions get bigger as you go down



115

Periodic Trends

- Across the period nuclear charge increases so they get smaller.
- Energy level changes between anions and cations



116

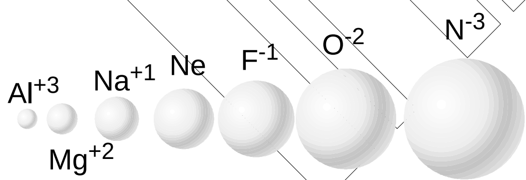
Size of Isoelectronic ions

- Iso - same
- Iso electronic ions have the same # of electrons
- Al^{+3} Mg^{+2} Na^{+1} Ne F^{-1} O^{-2} and N^{-3}
- all have 10 electrons
- all have the configuration $1s^2 2s^2 2p^6$

117

Size of Isoelectronic ions

- Positive ions have more protons so they are smaller



118

Electronegativity

119

Electronegativity

- The tendency for an atom to attract electrons to itself when it is chemically combined with another element.
- How “greedy”
- Big electronegativity means it pulls the electron toward itself.
- Atoms with large negative electron affinity have larger electronegativity.

120

Group Trend

- **The further down a group more shielding**
- **Less attracted (Z_{eff})**
- **Low electronegativity.**

121

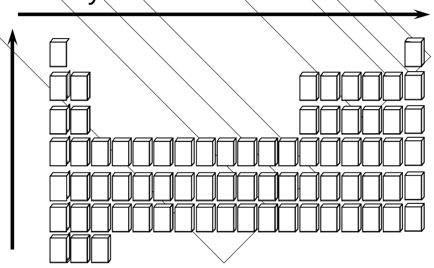
Periodic Trend

- **Metals are at the left end**
- **Low ionization energy- low effective nuclear charge**
- **Low electronegativity**
- **At the right end are the nonmetals**
- **More negative electron affinity**
- **High electronegativity**
- **Except noble gases**

122

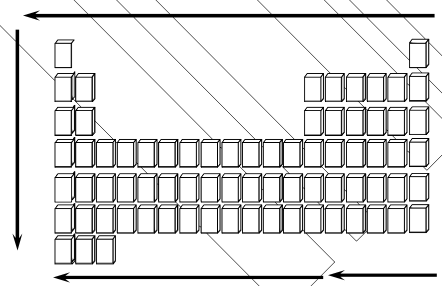
Ionization energy, electronegativity

Electron affinity INCREASE



123

Atomic size increases,



Ionic size increases

124

Parts of the Periodic Table

125

The information it hides

- **Know the special groups**
- **It is the number and type of valence electrons that determine an atom's chemistry.**
- **You can get the electron configuration from it.**
- **Metals lose electrons have the lowest IE**
- **Non metals- gain electrons most negative electron affinities**

126

The Alkali Metals

- Doesn't include hydrogen- it behaves as a non-metal
- decrease in IE
- increase in radius
- Decrease in density
- decrease in melting point
- Behave as reducing agents

127

Reducing ability

- Lower IE< better reducing agents
- Cs>Rb>K>Na>Li
- works for solids, but not in aqueous solutions.
- In solution Li>K>Na
- Why?
- It's the water -there is an energy change associated with dissolving

128

Hydration Energy

- $Li^+(g) \rightarrow Li^+(aq)$ is exothermic
- for Li^+ -510 kJ/mol
- for Na^+ -402 kJ/mol
- for K^+ -314 kJ/mol
- Li is so big because of it has a high charge density, a lot of charge on a small atom.
- Li loses its electron more easily because of this in aqueous solutions

129

The reaction with water

- Na and K react explosively with water
- Li doesn't.
- Even though the reaction of Li has a more negative ΔH than that of Na and K
- Na and K melt
- ΔH does not tell you speed of reaction
- More in Chapter 12.

130