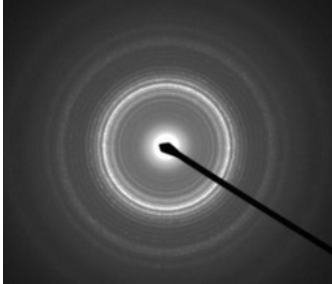
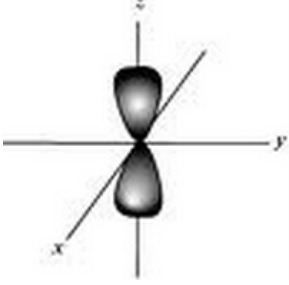


## A Much Closer Look at Atomic Structure

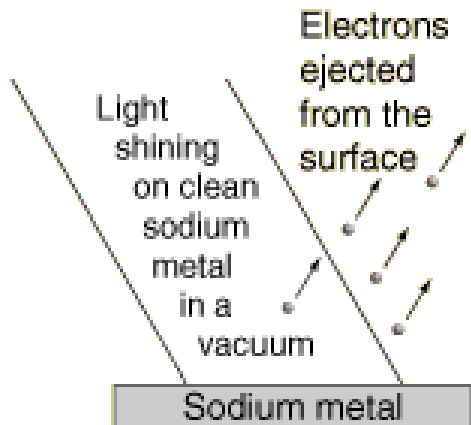
### Ideas We Will Clear Up Before You Graduate:

WRONG IDEAS	BETTER SUPPORTED BY EXPERIMENTS
<p>1. The electron always behaves as a particle.</p>	<p>1. There's a wavelength associated with very small particles like the electron, and it implies that the electron has both particle &amp; wave-like properties.</p> 
<p>2. There are orbits for electrons</p>	<p>2. There are areas where certain electrons are most likely to be. Those areas are obtained mathematically, but the electron's precise location cannot be pinned down.</p> 
<p>3. Electrons are arranged in shells. Electrons in the same shell are identical.</p>	<p>3. Shells don't exist. There is a principal <b>quantum</b> number corresponding to energy levels. Even within an energy level, every electron of an atom is different, having a unique set of four quantum numbers, including spin, which is involved in bonding and magnetism.</p>

The next 18 pages will clarify the above!

# A Much Closer Look at Atomic Structure

## 1. Photoelectric Effect

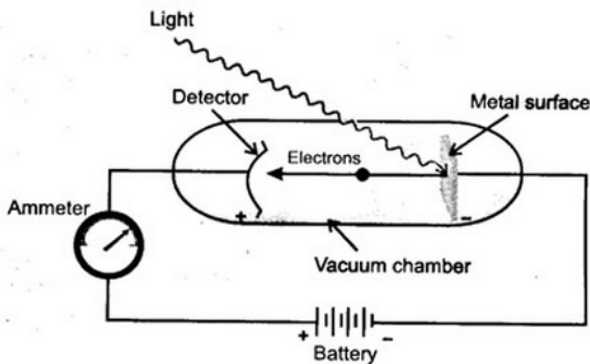


*This half-page was paraphrased from <http://hyperphysics.phy-astr.gsu.edu/hbase/mod1.html>*

- The details of the photoelectric effect were in direct contradiction to the expectations of very well developed classical physics.
- The explanation marked one of the major steps toward quantum theory.

- Mysteries of the photoelectric effect when it was first observed included:

- ? 1. The electrons were emitted immediately - no time lag!
- ? 2. Increasing the intensity of the light increased the number of electrons ejected by light, but not their maximum kinetic energy!
- ? 3. Red light did not cause the ejection of electrons, no matter what the intensity!
- ? 4. A weak violet light ejected only a few electrons, but their maximum kinetic energies was greater than those for intense light of longer wavelengths!



**Example 1** In the experimental setup of the photoelectric effect, does there have to be a gap between the metal surface and the detector?

## A Much Closer Look at Atomic Structure

Yes, otherwise the battery's voltage will cause electrons to flow, regardless of the light's effects. With the gap in place, electricity will only flow when the right light causes electrons to be ejected across the gap.

**Example 2** a) Will electrons be ejected from potassium metal if we use a bright, blinding 700 nm red light?

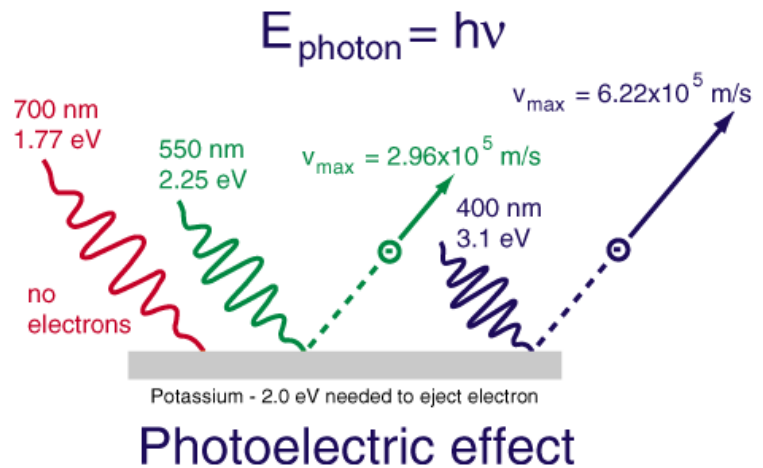
No

b) Will electrons be ejected from potassium metal with a 550 nm green light? Yes

c) Will electrons be ejected at a higher speed if we make the green light more intense & bright? No

If not, what will you observe instead?

We only get more photons, which implies that the energy of the photons is proportional to their frequency (and inversely proportional to their wavelength).



**Example 3** How did the concept of light have to be changed to account for the photoelectric effect?

It revealed that in certain experiments such as this one, the behaviour of light is like that of "particles" known as photons and not like those of waves. The energy of these photons is proportional to their frequency.

**Example 4** How can you use your hands to explain the difference between the intensity of photons of light versus the energy of photons?

A low-frequency photon (long wavelength such as red): hands open & close slowly

A high-frequency photon (short wavelength) : hands open & close quickly

A high-intensity, low frequency-photon: more hands opening & closing slowly

## A Much Closer Look at Atomic Structure

**Example 5** What relates the energy of a photon to its frequency? How are frequency & wavelength related?

TYPE OF energy	$\lambda$ =wavelength (m)* <sup>1</sup>	example of a $\lambda$ in that region; $\lambda$ =Wavelength(m)	$\nu$ = frequency (s <sup>-1</sup> )	Energy (Joules per photon)
<b>Radio</b>	$> 1 \times 10^{-1}$ (= 3 m for CHOM-FM)	3.0706	97700775.09	$6.47365 \times 10^{-26}$
<b>Microwave</b>	$1 \times 10^{-3} - 1 \times 10^{-1}$	0.01	30000000000	$1.9878 \times 10^{-23}$
<b>Infrared</b>	$7 \times 10^{-7} - 1 \times 10^{-3}$	0.0001	$3 \times 10^{12}$	$1.9878 \times 10^{-21}$
<b>Optical</b>	$4 \times 10^{-7} - 7 \times 10^{-7}$			
	<b>red 620–750 nm</b>	$6.85 \times 10^{-7}$	$4.37956 \times 10^{14}$	$2.9019 \times 10^{-19}$
	<b>orange 590–620 nm</b>	$6.05 \times 10^{-7}$	$4.95868 \times 10^{14}$	$3.28562 \times 10^{-19}$
	<b>yellow 570–590 nm</b>	$5.80 \times 10^{-7}$	$5.17241 \times 10^{14}$	$3.42724 \times 10^{-19}$
	<b>green 495–570 nm</b>	$6.32 \times 10^{-7}$	$4.74684 \times 10^{14}$	$3.14525 \times 10^{-19}$
	<b>blue 464–495 nm</b>	$4.72 \times 10^{-7}$	$6.35593 \times 10^{14}$	$4.21144 \times 10^{-19}$
	<b>indigo 450 - 464 nm</b>	$4.55 \times 10^{-7}$	$6.59341 \times 10^{14}$	$4.36879 \times 10^{-19}$
	<b>violet 400–450 nm</b>	$4.15 \times 10^{-7}$	$7.22892 \times 10^{14}$	$4.78988 \times 10^{-19}$
<b>UV = ultraviolet</b>	10 to 400 nm	$4.00 \times 10^{-8}$	$7.5 \times 10^{15}$	$4.965 \times 10^{-18}$
<b>X-ray</b>	$1 \times 10^{-11} - 1 \times 10^{-8}$	$1.00 \times 10^{-10}$	$3 \times 10^{18}$	$1.9878 \times 10^{-15}$
<b>Gamma-ray</b>	$< 1 \times 10^{-11}$	$1.00 \times 10^{-12}$	$3 \times 10^{20}$	$1.9878 \times 10^{-13}$

radio	=E/ $\nu$	= $6.47365 \times 10^{-26} \text{ J} / 97700775.09 \text{ s}^{-1} = 6.63 \times 10^{-34} \text{ Js}$
Orange light(visible)	=E/ $\nu$ = J/s <sup>-1</sup>	= $3.28562 \times 10^{-19} \text{ J} / 4.95868 \times 10^{14} \text{ s}^{-1} = 6.63 \times 10^{-34} \text{ Js}$

Note also  $\lambda\nu = c = \text{speed of light} = 3.00 \times 10^8 \text{ m/s}$

<sup>1</sup> What changes when light goes from one medium to another are both the *speed* of the light and the *wavelength* of the light. But the *frequency* of the series of light waves *does not change*; therefore, the color does not change. This implies that specific colors **are characterized by their frequencies**, not their wavelengths. It's why a colored plastic spoon appears the same color in water, even though it appears bent as light slows down.

## A Much Closer Look at Atomic Structure

### 2. Planck's Hypothesis

This hypothesis can explain the photoelectric effect by imagining light (and the entire electromagnetic spectrum) as being **quantized**, acting as if it came in discrete bundles.

The energy of the "bundle" is defined as

$$E = h\nu$$

*E = 1 photon's energy in Joules*

*h = Planck's constant =  $6.626176 \times 10^{-34}$  J s*

*$\nu$  = emission frequency of photon emission in  $s^{-1}$*

*( $s^{-1}$  means how many photons per second)*

*The first person to apply Planck's equation to the photoelectric effect was Albert Einstein in 1905. Sixteen years later, he was given the Nobel Prize for Physics, mostly for his work on the photoelectric effect.*

**Example 1** Does light only act as if it comes in quanta or "energy bundles"? What is the **complementary principle**? Does the latter apply to matter?

**No, it behaves as a wave in different experiments. Light consists of oscillating electrical and magnetic waves that do so at 90°.**

**The complementary principle, which also applies to matter: classical concepts like "particle" and "wave" cannot be used to fully describe the behavior of quantum-scale objects like photons and electrons.**

## A Much Closer Look at Atomic Structure

### 3. A) The Idea of Quanta Applied to Bohr's Model

When Bohr observed the discrete line spectrum of excited hydrogen gas, he realized that the electron's energy levels were quantized (meaning that only the electron could only move in certain discrete energy levels and not in between).

Use this following formula to figure out what colors are released by excited hydrogen atoms.

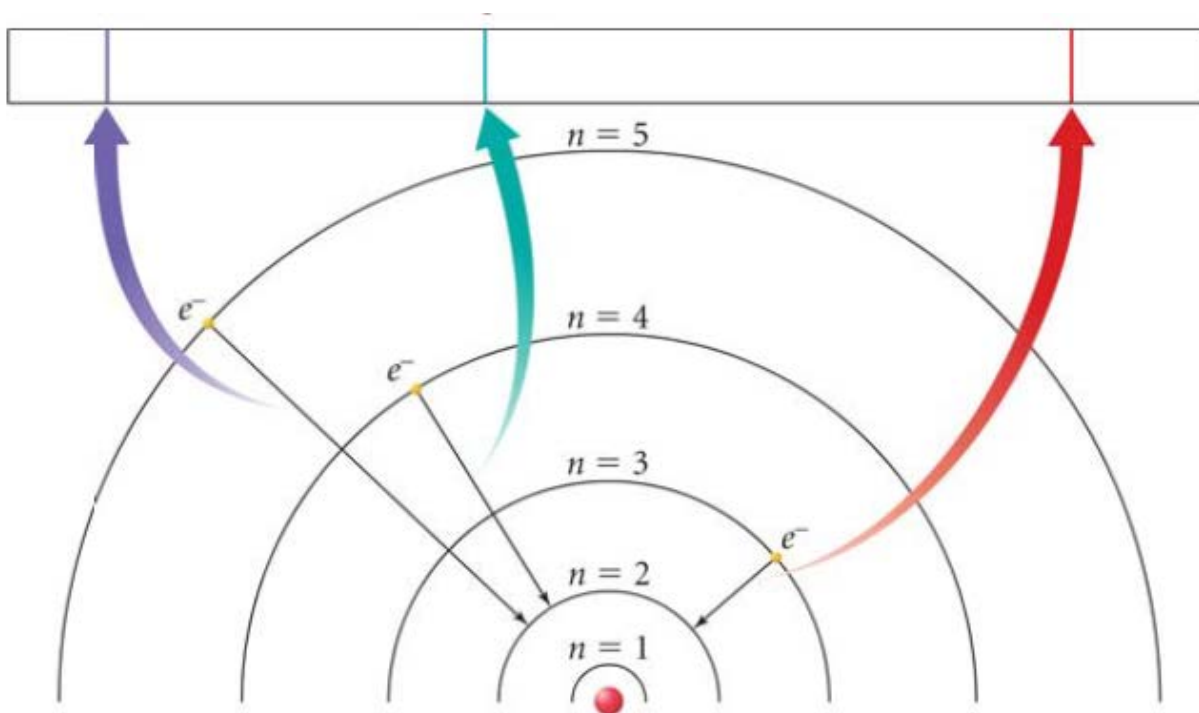
$$\Delta E = -2.178 \times 10^{-18} \text{ J} \left( \frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2} \right)$$

Where  $\Delta E$  = energy released when electron falls towards a lower energy level

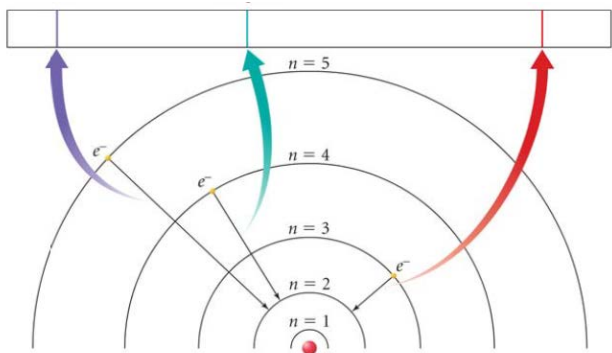
$Z$  = charge of nucleus

$n_f$  = higher energy level

$n_i$  = lower energy level



## A Much Closer Look at Atomic Structure



Show the sample calculation here for an n=5 to 2 transition, revealing why it's a violet line.

n = 5 to n = 2

$$\Delta E = -2.178 \times 10^{-18} \text{ J} \left( \frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2} \right)$$

$$\begin{aligned} \Delta E &= -2.178 \times 10^{-18} \text{ J} \left( \frac{1^2}{2^2} - \frac{1^2}{5^2} \right) = 0.21(2.178 \times 10^{-18}) \text{ J} \\ &= 4.57 \times 10^{-19} \text{ J} \end{aligned}$$

$$E = h\nu$$

$$\nu = \frac{E}{h} = 4.57 \times 10^{-19} \text{ J} / 6.626 \times 10^{-34} \text{ J s} = 6.90 \times 10^4 \text{ s}^{-1}$$

$$\lambda = c/\nu = (3.00 \times 10^8 \text{ m/s}) / 6.90 \times 10^4 \text{ s}^{-1} = 4.34 \times 10^{-7} \text{ m}$$

$4.34 \times 10^{-7} \text{ m} (10^9 \text{ nm/m}) = 434 \text{ nm} : \text{min violet range (see table on p142)}$

## A Much Closer Look at Atomic Structure

### 3. B) Derivation of: $\Delta E = -2.178 \times 10^{-18} J \left( \frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2} \right)$

The centripetal force between the electron and the nucleus is balanced by the coulombic attraction between them:

$$\frac{mv^2}{r} = \frac{Ze^2}{r^2}, \text{ where } Z = \text{atomic number and } e = \text{charge of electron}$$

$$mv^2 = \frac{Ze^2}{r}, \tag{1}$$

$$\text{so } r = \frac{Ze^2}{mv^2} \tag{2}$$

Since the electron's energy is characteristic of its orbit, the energy cannot be lost or gained. It is quantized. According to Bohr, the angular momentum of the electron is a whole number

multiple of  $\frac{nh}{2\pi}$ :

$mvr = \frac{nh}{2\pi}$ , where  $v$  = velocity of electron;  $m$  = mass of electron;  $h$  = Planck's constant

$$v = \frac{nh}{2\pi mr} \tag{3}$$



## A Much Closer Look at Atomic Structure

Substituting (3) into (2):

$$r = \frac{Ze^2}{m \left[ \frac{nh}{2\pi mr} \right]^2} = \frac{Ze^2 4\pi^2 m^2 r^2}{mn^2 h^2}$$

$$\frac{n^2 h^2}{4\pi^2 m Ze^2} = r$$

(4)

For the radius of hydrogen's atom

$$Z = 1$$

$$n = 1$$

$$h = 6.6262 \times 10^{-34} \text{ Js} = 6.6262 \times 10^{-34} \text{ kg m}^2/\text{s}^2 (\text{s}) = 6.6262 \times 10^{-34} \text{ kg m}^2/\text{s}$$

$$m = 9.1096 \times 10^{-31} \text{ kg}$$

$$e = 1.51899 \times 10^{-14} \text{ kg}^{0.5} \text{ m}^{1.5} \text{ s}^{-1}$$

$$r = \frac{1^2 (6.6262 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1})^2}{4\pi^2 (9.1096 \times 10^{-31} \text{ kg})(1)(1.51894 \times 10^{-14} \text{ kg}^{0.5} \text{ m}^{1.5} \text{ s}^{-1})^2} = 0.529 \times 10^{-10} \text{ m}$$

$$= 0.529 \text{ \AA}$$

The total energy of the electron is the sum of its kinetic and potential energies:

$$E_T = E_k + E_p$$

## A Much Closer Look at Atomic Structure

$$= mv^2/2 - Ze^2/r \tag{5}$$

Substituting (1) into (5):

$$E_T = Ze^2/2r - Ze^2/r$$

$$E_T = Ze^2/2r - 2Ze^2/2r$$

$$E_T = -Ze^2/2r \tag{6}$$

Substituting (4) into (6):

$$E_T = \frac{-Ze^2}{2\left(\frac{n^2 h^2}{4\pi^2 mZe^2}\right)} = \frac{-4\pi^2 mZ^2 e^4}{2n^2 h^2} = \frac{-2\pi^2 mZ^2 e^4}{n_o^2 h^2}$$

When an electron falls back to a lower energy level, it emits a photon of energy  $h\nu$  which is the difference in the energy between the energy outer level,  $E_o$  and that of the inner level,  $E_i$

$$h\nu = E_o - E_i = \left( \frac{-2\pi^2 mZ^2 e^4}{n_o^2 h^2} - \frac{-2\pi^2 mZ^2 e^4}{n_i^2 h^2} \right) =$$

## A Much Closer Look at Atomic Structure

$$= \frac{2\pi^2 m Z^2 e^4}{h^2} \left( \frac{1}{n_i^2} - \frac{1}{n_o^2} \right)$$

$$\frac{2\pi^2 m Z^2 e^4}{h^2} = \frac{2\pi^2 (9.1096 \times 10^{-31} \text{ kg})(1)^2 (1.51894 \times 10^{-14} \text{ kg}^{0.5} \text{ m}^{1.5} \text{ s}^{-1})^4}{(6.6262 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1})^2} =$$

$$= 2.178 \times 10^{-18} \text{ J}$$

### Exercises<sup>2</sup>

1.
  - a) In the photoelectric effect, something with particle-like properties knocks an electron from the surface of a metal. What is that "something" called?
  - b) If its frequency is too low, why will it not be able to knock off an electron?
2.
  - a) Calculate the energy of one photon of yellow light with a wavelength of 589 nm.
  - b) What if a mole of a specific metal absorbed a mole of photons at that same wavelength. How much energy would be absorbed by the metal?
3.
  - a) A certain laser emits light with a frequency of  $4.69 \times 10^{14} \text{ s}^{-1}$ . What is the energy of one photon from this laser?
  - b) What is the wavelength of this laser light's photons expressed in nm (nanometers;  $1 \text{ m} = 10^9 \text{ nm}$ )?
4. If a hydrogen electron "jumps" from the  $n=3$  to  $n=7$  level, will it emit or absorb energy?
5. Use the appropriate formula and table( in example 5) to identify the type of energy emitted when an excited hydrogen electron falls from  $n=2$  to  $n=1$ .
6. What is the **complementary principle**?
7. What characterizes a particular color? Its wavelength? Or frequency?

---

<sup>2</sup> **Answers:** 1. a)photon, b)no 2. a) $3.37 \times 10^{-19} \text{ J}$  b) $2.03 \times 10^5 \text{ J}$  3. a)  $3.11 \times 10^{-19} \text{ J}$  b)  $6.40 \times 10^2 \text{ nm}$  4. Absorb  
5.  $\nu = 2.47 \times 10^{15} \text{ s}^{-1}$ ;  $\lambda = 121 \text{ nm} = \text{UV}$

## A Much Closer Look at Atomic Structure

### 4. The Complementary Principle Applies to Matter: De Broglie

([http://chemwiki.ucdavis.edu/Physical\\_Chemistry/Quantum\\_Mechanics/Quantum\\_Theory/De\\_Broglie\\_Wavelength](http://chemwiki.ucdavis.edu/Physical_Chemistry/Quantum_Mechanics/Quantum_Theory/De_Broglie_Wavelength))

We have seen that depending on the experiment, light either demonstrates wave or particle-like (photons) behaviour. Can the same be true of matter, especially if it involves extremely small particles?

#### Deriving the De Broglie Wavelength

De Broglie derived his equation using well-established theories through the following series of substitutions:

1. He first used Einstein's famous equation relating matter and energy:

$$E = mc^2$$

with

$$E = \text{energy,}$$

$$m = \text{mass,}$$

$$c = \text{speed of light}$$

2. Using Planck's theory which states every quantum of a wave has a discrete amount of energy given by Planck's equation:

$$E = h\nu$$

3. Since de Broglie believed particles and wave have the same traits, he hypothesized that the two energies would be equal:

$$mc^2 = h\nu$$

4. Substitute an expression for frequency containing wavelength. Then, because real particles do not travel at the speed of light, De Broglie substituted velocity ( $v$ ) for the speed of light ( $c$ ).

**Example 1** From the above, derive an expression for the wavelength of a particle.

$$c = \lambda\nu.$$

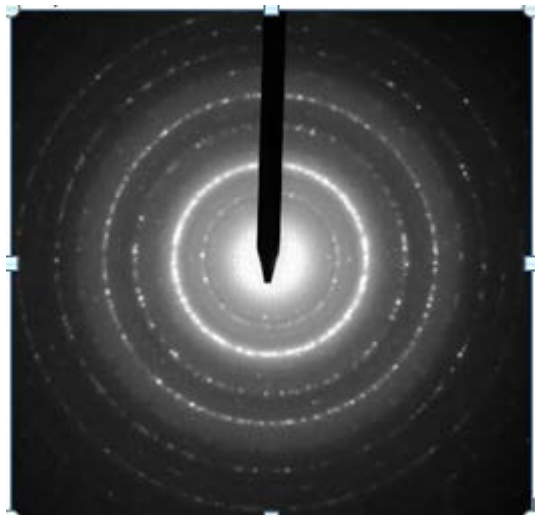
$$\nu = c/\lambda$$

$$mc^2 = h\nu$$

$$mc^2 = h c/\lambda$$

$$mc = h/\lambda$$

$$\lambda = h/mc.$$



Although De Broglie was credited for his hypothesis, he had no actual experimental evidence for his conjecture. In

## A Much Closer Look at Atomic Structure

1927, Clinton J. Davisson and Lester H. Germer shot electron particles onto a nickel crystal. What they see is the diffraction of the electron similar to waves diffraction against crystals (x-rays). In the same year, an English physicist, George P. Thomson fired electrons towards thin metal foil providing him with the same results as Davisson and Germer.

**Example 2** Find the de Broglie wavelength for an electron moving at the speed of  $6.63 \times 10^6$  m/s. (mass of an electron =  $9.11 \times 10^{-31}$  kg)

Handwritten calculation for Example 2:

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{9.11 \times 10^{-31} \text{ kg} \cdot (6.63 \times 10^6 \text{ m/s})} = 1.10 \times 10^{-10} \text{ m}$$

**Example 3** Which part of the electromagnetic radiation spectrum does the wavelength of the electron fall under?

Handwritten note: X-rays ( $1 \times 10^{-11}$  to  $1 \times 10^{-8}$  m) range

**Example 4** What would happen if you applied the deBroglie equation to a moving macroscopic object, like a car? Why is the wavelength the way it is—is it more because of its velocity relative to the electron’s or because of the car’s mass?

Handwritten calculation for Example 4:

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{2 \times 10^3 \text{ kg} \cdot 27.8 \text{ m/s}} = 1.19 \times 10^{-38} \text{ m}$$

Annotations: "mass is too big" (with an arrow pointing to the mass term) and "negligible" (with an arrow pointing to the final result).

## A Much Closer Look at Atomic Structure

### Exercises

1. What two basic physics laws are used to derive  $\Delta E = -2.178 \times 10^{-18} J \left( \frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2} \right)$   
(see p146)
2. Use  $E = mc^2$  and  $E = h\nu$  to derive the expression that Broglie used to find the wavelength of the electron.
3. Beta particles, which are emitted by some radioactive materials and the innermost electrons of atoms of elements having large atomic number, such as gold move much faster than the electron of hydrogen. Specifically, gold's innermost electrons move at 58% of the speed of light, and instead of the typical  $< 0.01c$  for a hydrogen atom's electron.  
Calculate the wavelength of an innermost electron in both cases.

... laws are used to derive  $\Delta E = -2.178 \times 10^{-18} J \left( \frac{Z^2}{n_f^2} - \frac{Z^2}{n_i^2} \right)$   
*equating centripetal force with Coulomb's law*  
 Use  $E = mc^2$  and  $E = h\nu$  to derive the expression that Broglie used to find the wavelength of the electron.  
*see p 150*

3. Beta particles, which are emitted by some radioactive materials and the innermost electrons of atoms of elements having large atomic number, such as gold move much faster than the electron of hydrogen. Specifically, gold's innermost electrons move at 58% of the speed of light, and instead of the typical  $< 0.01c$  for a hydrogen atom's electron.  
 Calculate the wavelength of an innermost electron in both cases.

*see p 151*       $\lambda = \frac{h}{mc}$

=

hydrogen's $e^-$ : $0.01c$	gold $0.58c$
$\lambda = \frac{6.626 \times 10^{-34}}{9.11 \times 10^{-31} \text{ kg} (0.01 * 3 \times 10^8)}$	$\frac{6.626 \times 10^{-34}}{9.11 \times 10^{-31} (0.58 * 3 \times 10^8)}$
$= 2.42 \times 10^{-10} \text{ m}$	$4.18 \times 10^{-12} \text{ m}$

## A Much Closer Look at Atomic Structure

### 5. The Quantum Mechanical Model of the Atom

#### A- Schrodinger's Wave Function and the Uncertainty Principle

Although the concept of energy levels encountered in the Bohr model was in some way accurate, once deBroglie revealed the electron's wave-particle duality, a new model of the atom was needed. Electrons do not move in circular orbits.

**Schrodinger** came with a complex mathematical equation involving a 3-D operator, a wave function and the energy of electrons. Different solutions to the equation were specific wave functions known as orbitals.

The movement of the electron cannot be tracked with exact position due to its wave-particle duality. There is a minimum uncertainty in its product of momentum,  $p$ , and position,  $x$ , given by the **Heisenberg uncertainty principle**:

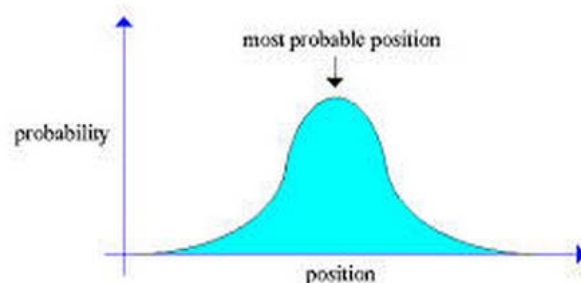
$$\Delta x(\Delta p) \geq \frac{h}{4\pi} \quad \text{Notice our buddy, } h, \text{ the Planck constant, appearing again!}$$

**Example 1:** What is an electron orbital?

It's a wave function that happens to be a mathematical solution to the Schrodinger equation.

**Example 2:** Show that the units are compatible in the expression for Heisenberg uncertainty principle.

Quantum Wave Function



ple.

$$\Delta x (\Delta p) \quad \Delta p = m \Delta v$$

$$m \rightarrow \left( \frac{h \cdot m}{s} \right) \quad h$$

$$\left| \frac{h \cdot m^2}{s} \right| = \frac{h \cdot m}{s} \cdot m \quad \text{mad}$$

## A Much Closer Look at Atomic Structure

**Example 3:** a) From the uncertainty principle, calculate  $\Delta x$  for an electron with uncertainty in

$$m\Delta v = \Delta p = 9.1096 \times 10^{-31} (0.100) = 9.1096 \times 10^{-32}$$

$$\Delta x (\Delta p) \geq \frac{h}{4\pi} \rightarrow \geq 5.79 \times 10^{-4} \text{ m}$$

$$\Delta x \geq \frac{h}{\Delta p 4\pi} \geq \frac{6.626 \times 10^{-34} \text{ J s}}{9.1096 \times 10^{-32} \cdot 4 \cdot 3.1415}$$

momentum that comes from an uncertainty in velocity  $\Delta v = \pm 0.100 \text{ m/s}$ .  
(Momentum =  $p = m \Delta v$ ; mass of electron =  $9.1096 \times 10^{-31} \text{ kg}$ )

b) How does  $\Delta x$  compare to the size of a hydrogen atom ( $1 \times 10^{-10} \text{ m}$ )

$\Delta x$  is much bigger, meaning that the uncertainty in position is huge!

### B- The Square of the Wave Function and Quantum Numbers

If we take the square of the wave function, we get solutions that represent a high probability of finding an electron in a certain area. For example, there is a 90% chance of finding a hydrogen electron in its unexcited state, the so-called s-orbital.

*The Solutions to the Schrodinger Equation*

$n$	$L$	Orbital designation	$m_l$	Number of orbitals	Number of electrons per orbital
1	0	1s	0	1	2
2	0	2s	0	1	2
	1	2p	-1, 0, 1	3	6
3	0	3s	0	1	2
	1	3p	-1, 0, 1	3	6
	2	3d	-2, -1, 0, 1, 2	5	10
4	0	4s	0	1	2
	1	4p	-1, 0, 1	3	6
	2	4d	-2, -1, 0, 1, 2	5	10
	3	4f	-3, -2, -1, 0, 1, 2, 3	7	14

*Handwritten notes: 'Angular momentum quantum number' is written vertically in the L column. 'Orbital designation' is written vertically in the 3rd column. 'm\_l' is written vertically in the 4th column. 'Number of orbitals' is written vertically in the 5th column. 'Number of electrons per orbital' is written vertically in the 6th column. There are also handwritten 'n' and 'l' labels near the first few rows.*

**Example 1:** Fill in the table above.

**Example 2:** What corresponds to the number of electrons per orbital type in the periodic table? Hint: see blocks It's equal to the number of elements in each block



## A Much Closer Look at Atomic Structure

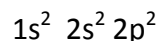
**Example 3:** For  $n = 5$ , give the allowed number of  $l$  values and the orbital designation of each value.

$$n=5, \text{ so } l = 0 \text{ to } n-1 \text{ or } 0 \text{ to } 4 \text{ or } 0,1,2,3,4 = 5s, 5p, 5d, 5f, 5g$$

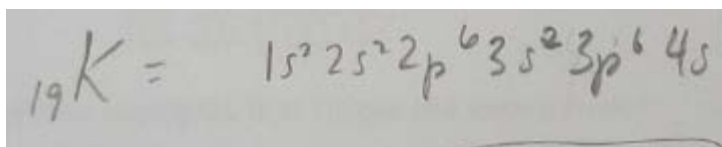
**Example 4:** Is there a simple formula relating the total number of electrons that can have a certain principle quantum number,  $n$ ? Think of it.

$$= 2n^2$$

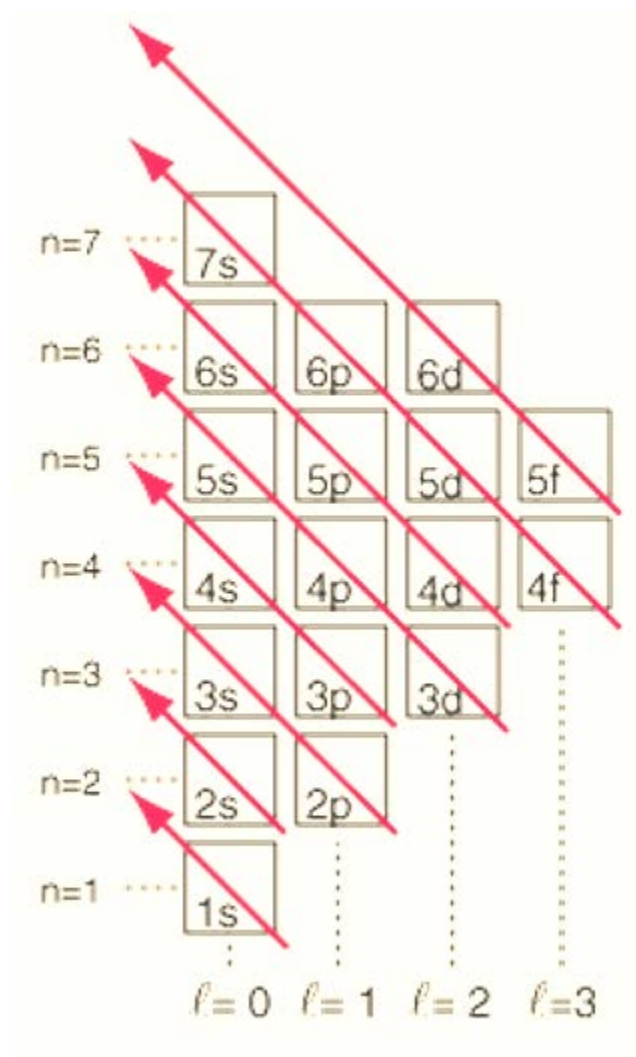
**Example 5:** Here's the order in which electrons fill the orbitals, followed by the electron configuration for carbon:



What is the electron configuration for **potassium**?



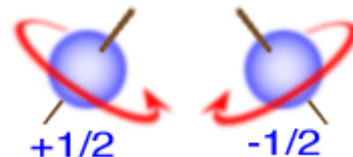
**Example 6:** What is the electron configuration for **cadmium** ( $_{48}\text{Cd}$ )?



## A Much Closer Look at Atomic Structure

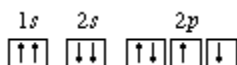
### C- Rules For Electron Configuration: the Box Method

1. **Aufbau Principle:** electrons fill orbitals starting at the lowest available energy state before filling higher states (1s before 2s; 2p before 3 p etc).
2. **Hund's Rule:** When filling sublevels other than s, electrons are placed in individual orbitals before they are paired up.
3. **Pauli Exclusion Principle:** When we draw electrons, we use up and down arrows. So, if an electron is paired up in a box, one arrow is up and the second must be down.

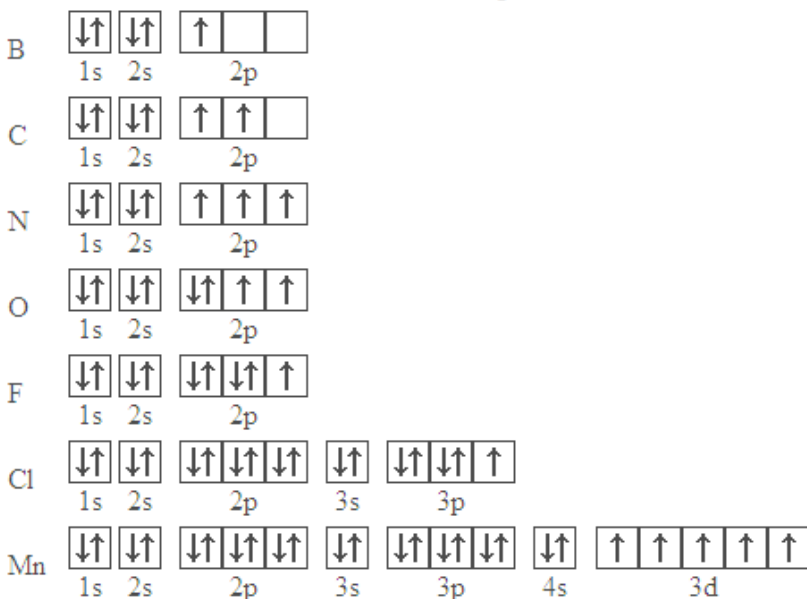


This is because no two electrons in the same atom can have the same set of four quantum numbers. An orbital can hold 0, 1, or 2 electrons only, and if there are two electrons in the orbital, they must

have opposite (paired) spins; like this  $\begin{array}{c} 1s \\ \uparrow\downarrow \end{array}$   $\begin{array}{c} 2s \\ \uparrow\downarrow \end{array}$   $\begin{array}{c} 2p \\ \uparrow\downarrow \uparrow \uparrow \end{array}$  and **not** like this

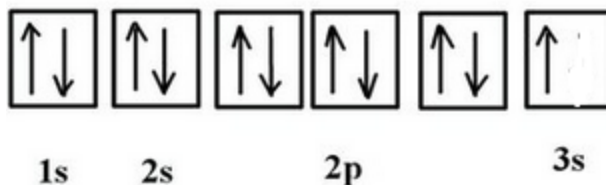


Some examples that follow the above rules:

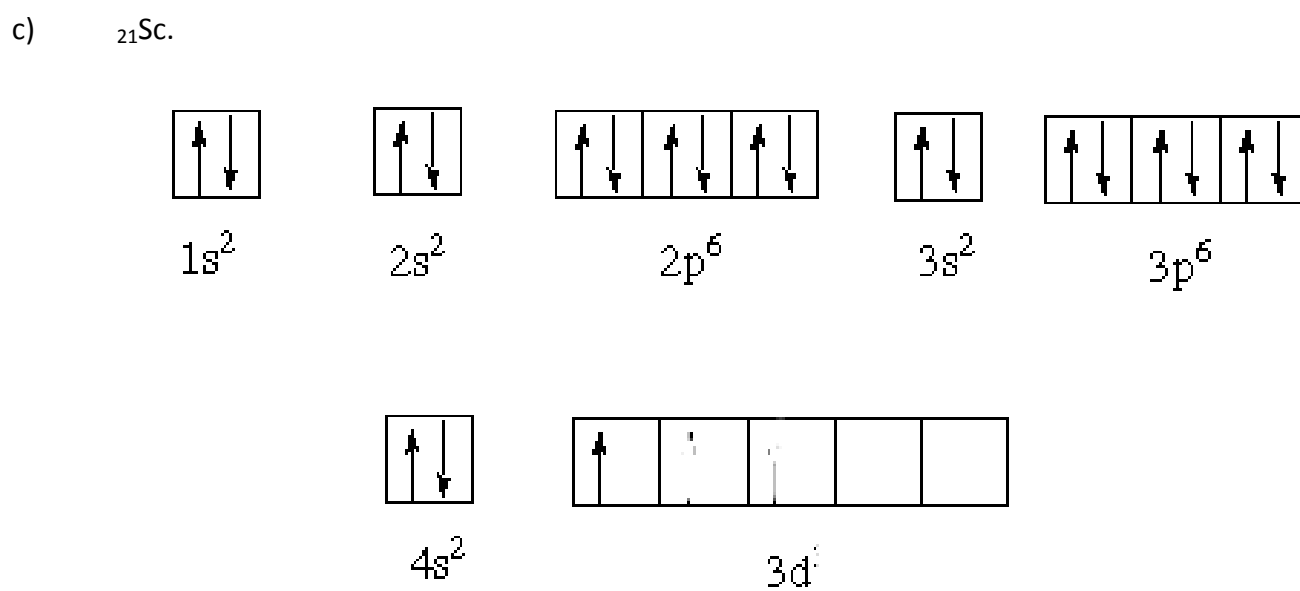
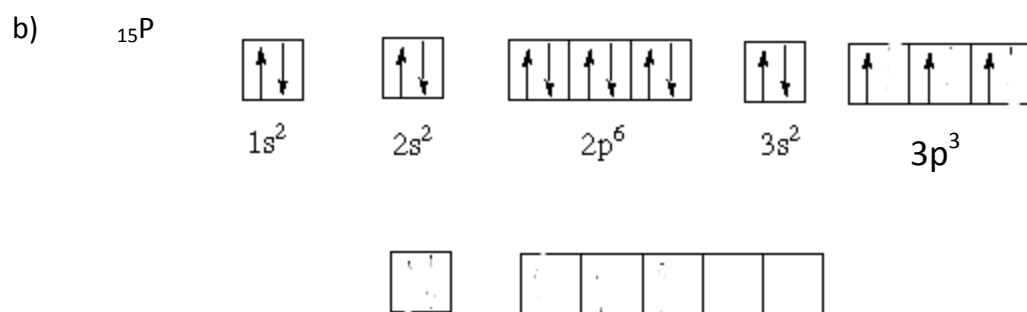


**Example 1** Use the box (or circle method) to show the electron configuration of

a)  ${}_{11}\text{Na}$

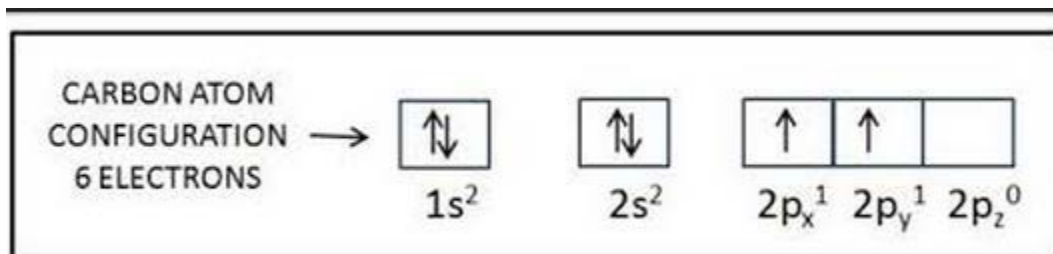


## A Much Closer Look at Atomic Structure



## A Much Closer Look at Atomic Structure

**Example 2:** What are the quantum numbers assigned to each of carbon's 6 electrons?



n	L= up to n-1	Orbital designation	M <sub>l</sub> from 0 to +/- L	Number of orbitals	Number of electrons per orbital
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**n, L, m, s**

**1s<sup>2</sup> guys:**    **1,0,0, +1/2 and 1,0,0, -1/2**

**2s<sup>2</sup> guys:**    **2,0,0, +1/2 and 2,0,0, -1/2**

**2p<sup>2</sup> guys**     **2,1,-1, +1/2 and 2,1,0, +1/2**

**Notice the same +1/2 for the two p electrons, but different orbitals: -1, 0**

### Exercises

1.    a) From the uncertainty principle, calculate  $\Delta x$  for a baseball with uncertainty in momentum that comes from an uncertainty in velocity  $\Delta v = \pm 0.100 \text{ m/s}$ .  
(Momentum =  $p = m \Delta v$ ; mass of baseball = 145 g)
  - b)    How does  $\Delta x$  compare to the size of a baseball (23.0 cm in diameter)
  
2.    a) What orbital characteristic does the *angular momentum* quantum number affect?  
**b)** Normally we assign letters to the angular momentum numbers of 0,1,2 and 3. What are the orbital's matching letters?
  
3.    Which quantum number gives you the number of orbitals for s, p,d or f?

## A Much Closer Look at Atomic Structure

Heisenberg uncertainty principle, calculate  $\Delta x$  for a baseball moving with a velocity uncertainty  $\Delta v = \pm 0.100 \text{ m/s}$ .  
 ( $\Delta v$ ; mass of baseball = 145 g)  $\Delta x \geq \frac{h}{m\Delta v} \geq \frac{6.62 \times 10^{-34}}{145 \times 10^{-3} \times 0.10 \times 4 \times 3.14159}$

Compare to the size of a baseball (23.0 cm in diameter)  $\geq 3.63 \times 10^{-33}$   
*much smaller! It's insignificant*

Which characteristic does the *angular momentum* quantum number affect? *type of orbital*  
 Letters to the angular momentum numbers of 0, 1, 2 and 3. What letters?  
 $0 = s$        $2 = d$   
 $1 = p$        $3 = f$

Which quantum number gives you the number of orbitals for s, p, d or f?  $\rightarrow m = 0 \rightarrow \neq l$   
 Write the quantum numbers for Na's 11 electrons.  
 Write the electron configurations (show orbitals and electron spins) for

4. Give the complete set of quantum numbers for Na's 11 electrons.

n	l	m	s	
1	0	0	$+\frac{1}{2}$	} $1s^2$
1	0	0	$-\frac{1}{2}$	
2	0	0	$+\frac{1}{2}$	} $2s^2$
2	0	0	$-\frac{1}{2}$	
2	1	-1	$+\frac{1}{2}$	} $2p^6$
2	1	0	$+\frac{1}{2}$	
2	1	1	$+\frac{1}{2}$	
2	1	-1	$-\frac{1}{2}$	
2	1	1	$-\frac{1}{2}$	
2	1	0	$-\frac{1}{2}$	

3	0	0	$+\frac{1}{2}$
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↑  
3s<sup>1</sup>

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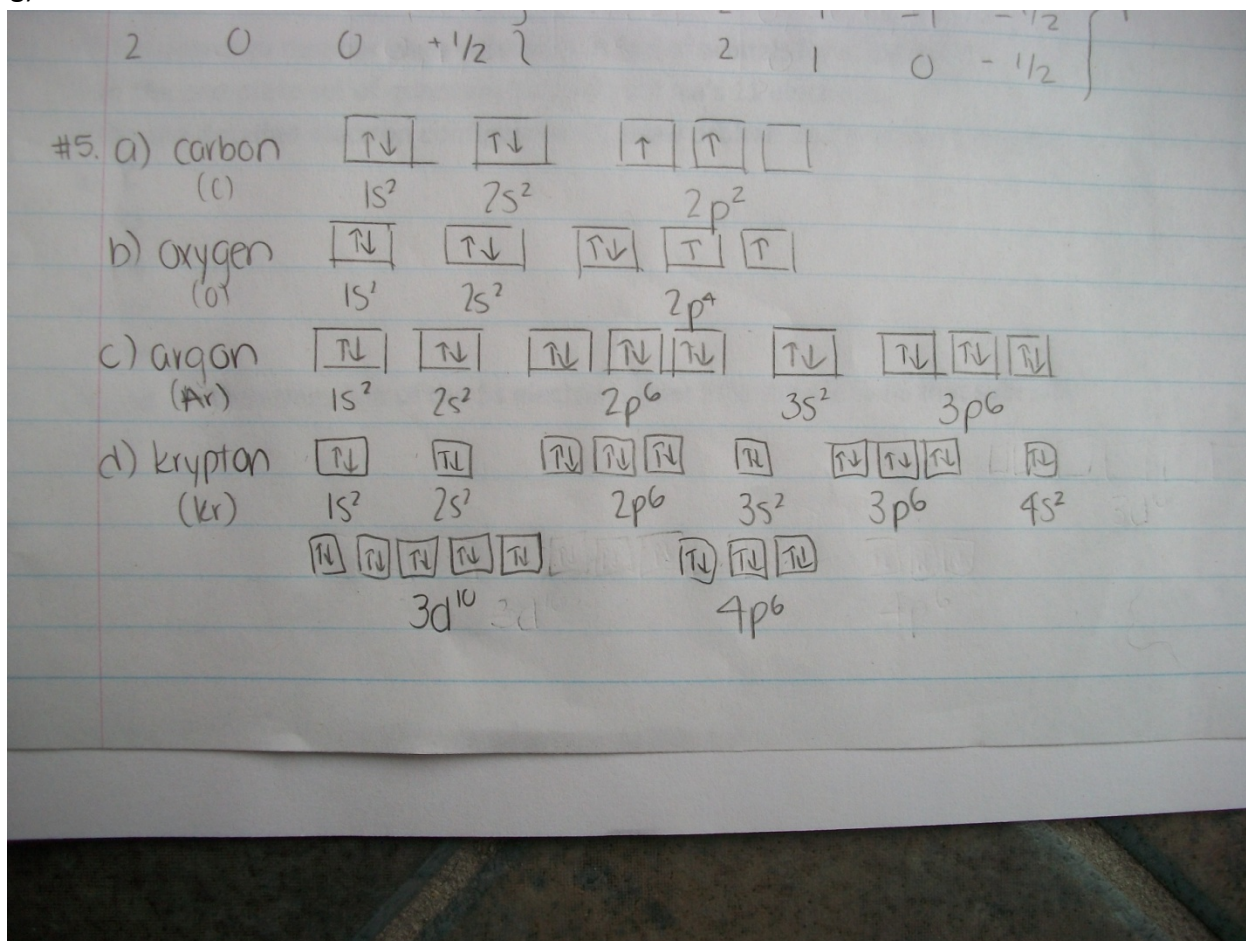
5. Write the detailed electron configurations (show orbitals and electron spins) for

- a) C
- b) O
- c) Ar
- d) Kr
- e) Fe

## A Much Closer Look at Atomic Structure

f) Ag (in this one, one of the 5s electrons goes into the d's to fill that sublevel.

g) Ir



More on the next page....



## A Much Closer Look at Atomic Structure

