CHAPTER 5

- The Structure of Atoms

Chapter Outline

Subatomic Particles

- Fundamental Particles
- The Discovery of Electrons
- Canal Rays and Protons
- Rutherford and the Nuclear Atom
- Atomic Number
- Neutrons
- Mass Number and Isotopes
- Mass spectrometry and Isotopic Abundance

9. The Atomic Weight Scale and Atomic Weights

Chapter Goals

The Electronic Structures of Atoms

- Electromagnetic radiation
- The Photoelectric Effect
- Atomic Spectra and the Bohr Atom
- The Wave Nature of the Electron
- The Quantum Mechanical Picture of the Atom
- Quantum Numbers
- Atomic Orbitals
- Electron Configurations
- Paramagnetism and Diamagnetism
- The Periodic Table and Electron Configurations

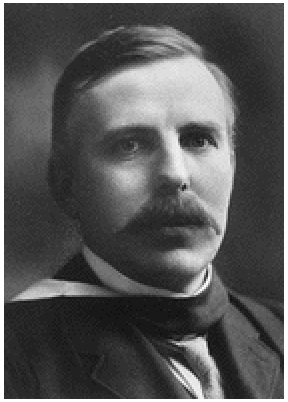
Fundamental Particles

- **Reading Assignment:** Please read from 5-1 to 5-4.
- Three fundamental particles make up atoms. The following table lists these particles together with their masses and their charges.

Particle	Mass (amu)	Charge	Discoverer
Electron (e^-)	0.00054858	-1	Davy (1800's) + others
Proton (p,p^+)	1.0073	+1	Goldstein (1886)
Neutron(n,n^0)	1.0087	0	Chadwick (1932)

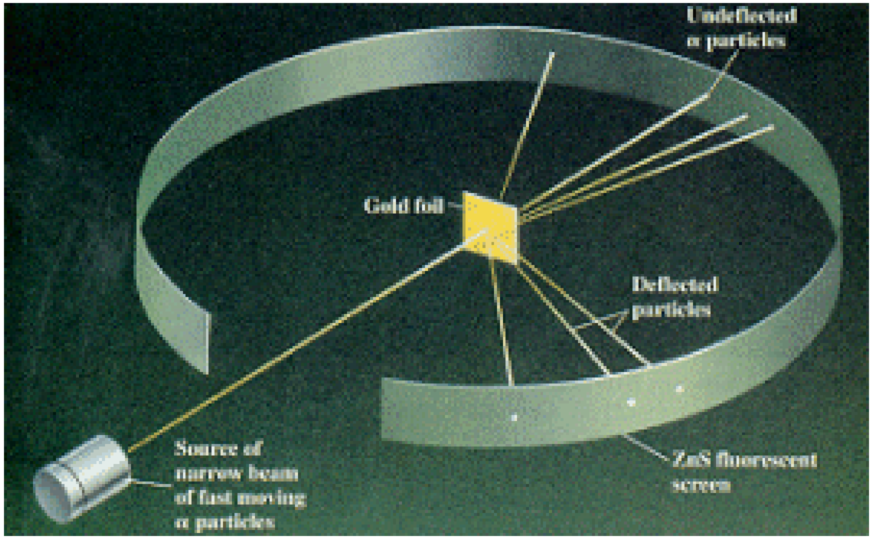
Rutherford and the Nuclear Atom

- In 1910, the research group of Ernest Rutherford ran a most important experiment now called the Rutherford Scattering Experiment, in which a piece of thin gold foil was bombarded with alpha (α) particles (products of radioactive decay).
  - alpha particle $\equiv$ He nucleus (atom minus its 2 electrons)
  - ${}^{2}_{4}He^{2+}$ (it has a 2+ charge)



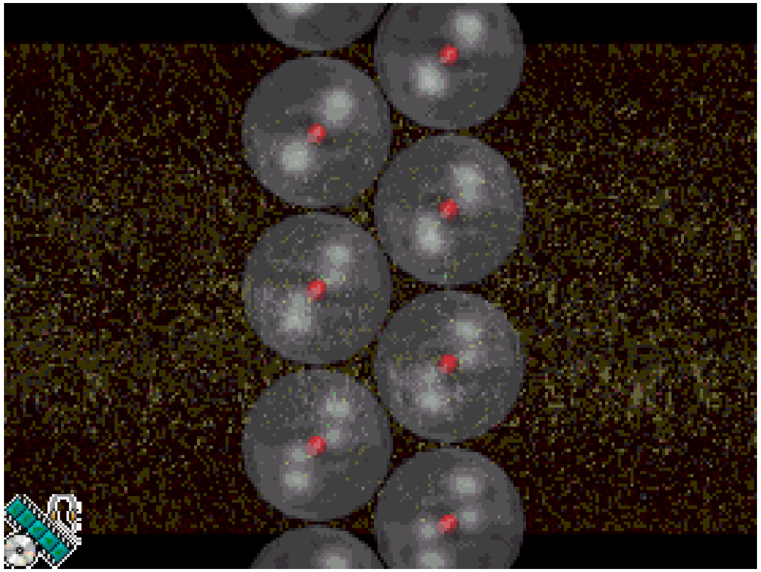
Rutherford and the Nuclear Atom

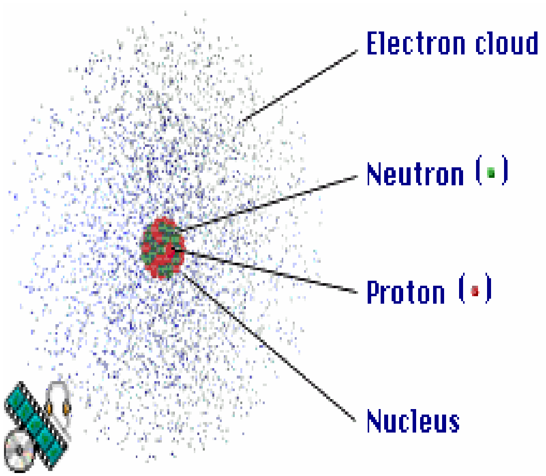
Most of the positively charged particles passed through the foil (that was expected); but some were deflected by the foil and a few bounced almost straight back. (Surprise!!!) What did this mean?



Rutherford and the Nuclear Atom

- Rutherford explanation involved a nuclear atom with electrons surrounding the nucleus .





Rutherford and the Nuclear Atom

- Rutherford's major conclusions from the α-particle scattering experiment

1. The atom is mostly empty space.
2. It contains a very small, dense center called the nucleus.
3. Nearly all of the atom's mass is in the nucleus.
4. The charge on the nucleus is positive
5. The nuclear diameter is 1/10,000 to 1/100,000 times less than atom's radius.

Atomic Number

- The atomic number (z) is equal to the number of protons in the nucleus.
  - On the periodic table Z is the uppermost number in each element's box.
- In 1913, H.G.J. Moseley realized that the atomic number determines the element .
  - The elements differ from each other by the number of protons in the nucleus.
  - The number of electrons in a neutral atom ("neutral" means the atom has no charge) is also equal to the atomic number.

Atoms

- **Problem:** Find the thickness of the gold foil (units: number of Au atoms)

Data: mass of sheet: 0.0893 g

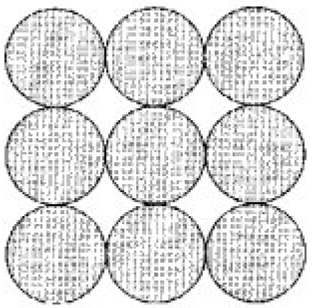
size of sheet: 14.0 cm x 14.0 cm

density of Au: 19.32 g/cm^3

diameter of Au atom: 2.8841 Å (1 Å = 10-10 m)

Au crystallizes in a cubic lattice

∴ packing of atoms is →



Simple Cubic Packing

Successive layers are superimposed over the base

Neutrons

- James Chadwick in 1932 analyzed the results of α-particle scattering on thin Be films.
- Chadwick recognized existence of massive neutral particles which he called neutrons.
  - Atoms consist of very small, very dense nuclei surrounded by clouds of electrons at relatively great distances from the nuclei. All nuclei contain protons; nuclei of all atoms except the common form of hydrogen also contain neutrons

Mass Number and Isotopes

- **Mass number (A)** is the sum of the number of protons and neutrons in the nucleus. (mass number is NOT atomic weight)
  - Z = proton number N = neutron number
  - A = Z + N
- A common symbolism used to show mass and proton numbers is

$^{A}_{Z}E$ where E = element symbol

A = mass number (# p + # n)

Z = atomic number (# p)

Mass Number and Isotopes

$$^{A}_{Z}E \text{ for example } ^{12}_{6}C,\ ^{48}_{20}Ca,\ ^{197}_{79}Au$$

- Can be shortened to this symbolism.

$$^{14}N,\ ^{63}Cu,\ ^{107}Ag, \text{ etc.}$$

Example: for ^{63}Cu, what is the number of protons, electrons, and neutrons?

p = 29 (look on periodic table)

e = 29 (# p = # e for a neutral atom)

n = A – Z = 63 – 29 = 34

Mass Number and Isotopes

- **Isotopes** are atoms of the same element but with different neutron numbers.
  - Isotopes have different masses and A values but are the same element.
- One example of an isotopic series is the hydrogen isotopes.

  ^{1}H or **protium** is the **most common** hydrogen isotope.
  - one proton, one electron, and **NO neutrons**

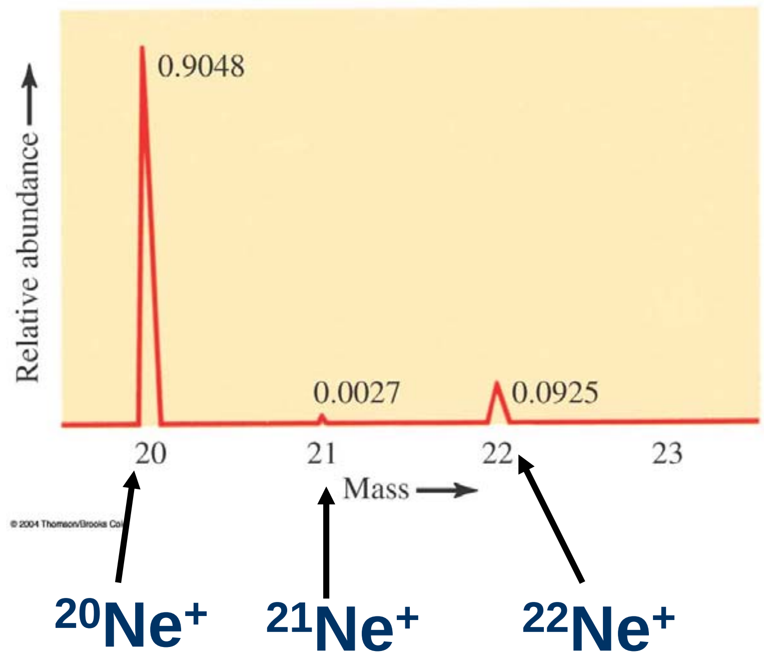
  ^{2}H or **deuterium** is the **second most abundant** hydrogen isotope.
  - one proton, one electron, and **ONE neutron**

  ^{3}H or **tritium** is a **radioactive** hydrogen isotope.
  - one proton, one electron, and **TWO** neutrons

Mass Number and Isotopes

- Some elements have only one isotope (F, I), but most elements occur in nature as mixtures of isotopes. The naturally occurring abundances of isotopes (table 5-3) are determined by **mass spectrometry**.

mass spectrometer



The Atomic Weight Scale and Atomic Weights

- If we define the mass of ${}^{12}_{6}C$, a specific isotope of C, as exactly 12 atomic mass units (amu), then it is possible to establish a relative weight scale for atoms.

  – 1 amu = (1/12) mass of ${}^{12}_{6}C$ by definition

Recall: since mass of one ${}^{12}_{6}C$ atom = 12 amu

mass of one mole of ${}^{12}_{6}C$ atoms = 12.0000g

The Atomic Weight Scale and Atomic Weights

- The **atomic weight** of an element is the **weighted average of the masses of its stable isotopes**

- **Example:** Naturally occurring **Cu** consists of **2 isotopes**. It is **69.1%** ^{63}Cu with a mass of **62.9 amu**, and **30.9%** ^{65}Cu, which has a mass of **64.9 amu**. Calculate the atomic weight of Cu to one decimal place.

The Atomic Weight Scale and Atomic Weights

The atomic weight of Cu:

$$\text{atomic weight} = \underbrace{(0.691)(62.9\text{ amu})}_{^{63}\text{Cu isotope}} + \underbrace{(0.309)(64.9\text{ amu})}_{^{65}\text{Cu isotope}}$$

$$\text{atomic weight} = 63.5\text{ amu for copper}$$

The Atomic Weight Scale and Atomic Weights

- **Example:** Naturally occurring chromium consists of four isotopes. It is 4.31% $_{24}^{50}Cr$, mass = 49.946 amu, 83.76% $_{24}^{52}Cr$, mass = 51.941 amu, 9.55% $_{24}^{53}Cr$, mass = 52.941 amu, and 2.38% $_{24}^{54}Cr$, mass = 53.939 amu. Calculate the atomic weight of chromium.

You do it!

The Atomic Weight Scale and Atomic Weights

The atomic weight of chromium:

$$
\begin{aligned}
\text{atomic weight} &= (0.0431 \times 49.946\ \text{amu}) + (0.8376 \times 51.941\ \text{amu}) \\
&\quad + (0.0955 \times 52.941\ \text{amu}) + (0.0238 \times 53.939\ \text{amu}) \\
&= \left(2.153 + 43.506 + 5.056 + 1.284\right)\text{amu} \\
&= 51.998\ \text{amu}
\end{aligned}
$$

The Atomic Weight Scale and Atomic Weights

- **Example:** **The atomic weight of boron is 10.811 amu. The masses of the two naturally occurring isotopes $_5^{10}B$ and $_5^{11}B$, are 10.013 and 11.009 amu, respectively. Calculate the fraction and percentage of each isotope.**

You do it!

- **This problem requires a little algebra.**
  - **A hint for this problem is $x + (1-x) = 1$**

The Atomic Weight Scale and Atomic Weights

The fraction and percentage of each isotope:

$$10.811\,\text{amu} = \underbrace{x(10.013\,\text{amu})}_{^{10}\text{B isotope}} + \underbrace{(1-x)(11.009\,\text{amu})}_{^{11}\text{B isotope}}$$

$$= (10.013\,x + 11.009 - 11.009\,x)\,\text{amu}$$

$$(10.811 - 11.009)\,\text{amu} = (10.013\,x - 11.009\,x)\,\text{amu}$$

$$-0.198 = -0.996\,x$$

$$0.199 = x$$

The Atomic Weight Scale and Atomic Weights

- Note that because x is the multiplier for the ^{10}B isotope, our solution gives us the fraction of natural B that is ^{10}B.
- Fraction of $^{10}B = 0.199$ and % abundance of $^{10}B = 19.9\%$.
- The multiplier for ^{11}B is $(1-x)$ thus the fraction of ^{11}B is $1-0.199 = 0.811$ and the % abundance of ^{11}B is 81.1%.

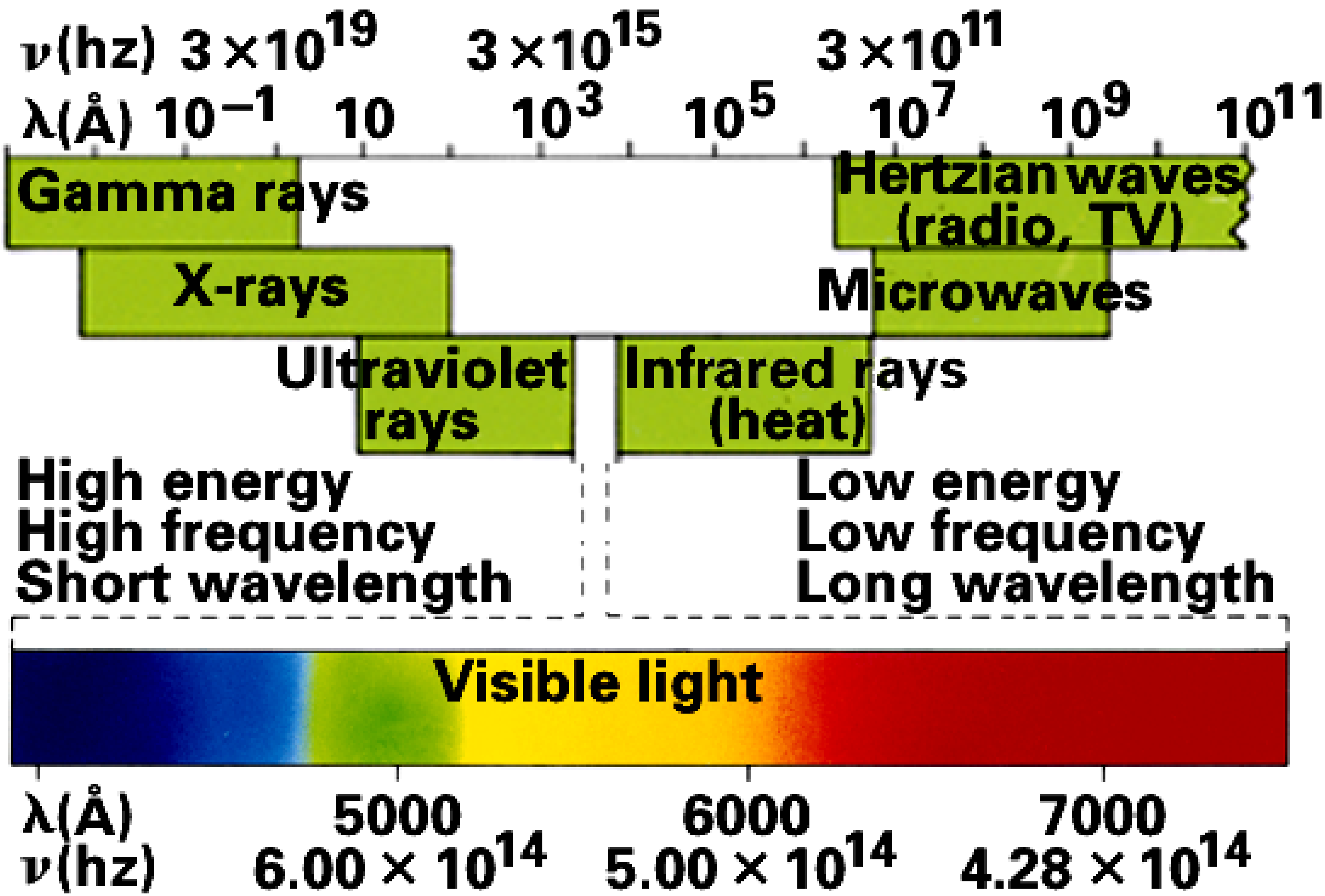
The Electronic Structures of Atoms
Electromagnetic Radiation

- The **wavelength** of electromagnetic radiation has the symbol λ .
- Wavelength is the distance from the top (crest) of one wave to the top of the next wave.
  - Measured in units of distance such as m,cm, Å.
  - 1 Å = 1×10^{-10} m = 1×10^{-8} cm
- The **frequency** of electromagnetic radiation has the symbol υ.
- Frequency is the number of crests or troughs that pass a given point per second.
  - Measured in units of 1/time - s^{-1}

Electromagnetic Radiation

- **The relationship between wavelength and frequency for any wave is velocity = λ υ.**
- **For electromagnetic radiation the velocity is 3.00 x 10^8 m/s and has the symbol c.**
- **Thus c = λ υ for electromagnetic radiation.**

Electromagnetic Radiation



Electromagnetic Radiation

- **Molecules interact with electromagnetic radiation.**
  - **Molecules can absorb and emit light.**
- **Once a molecule has absorbed light (energy), the molecule can:**
  1. **Rotate**
  2. **Translate**
  3. **Vibrate**
  4. **Electronic transition**

Electromagnetic Radiation

- **Example:** **What is the frequency of green light of wavelength 5200 Å?**

$$c = \lambda \nu \quad \therefore \quad \nu = \frac{c}{\lambda}$$

$$(5200\ \text{Å}) \left(\frac{1 \text{ x } 10^{-10}\ \text{m}}{1\ \text{Å}} \right) = 5.200 \times 10^{-7}\ \text{m}$$

$$\nu = \frac{3.00 \times 10^{8}\ \text{m/s}}{5.200 \times 10^{-7}\ \text{m}}$$

$$\nu = 5.77 \times 10^{14}\ \text{s}^{-1}$$

Electromagnetic Radiation

- In 1900 **Max Planck** studied black body radiation and realized that to explain the energy spectrum he had to assume that:
  1. energy is quantized
  2. light has particle character
- Planck's equation is

$$E = h\nu \quad \text{or } E = \frac{hc}{\lambda}$$

$$h = \text{Planck's constant} = 6.626 \text{ x } 10^{-34} \text{ J} \cdot \text{s}$$

Electromagnetic Radiation

- **Example: What is the energy of a photon of green light with wavelength 5200 Å? What is the energy of 1.00 mol of these photons?**

$$\text{We know that } \nu = 5.77 \text{ x } 10^{14} \text{ s}^{-1}$$

$$\text{E} = \text{h}\,\nu$$

$$\text{E} = (6.626 \times 10^{-34} \text{ J} \cdot \text{s})(5.77 \times 10^{14} \text{ s}^{-1})$$

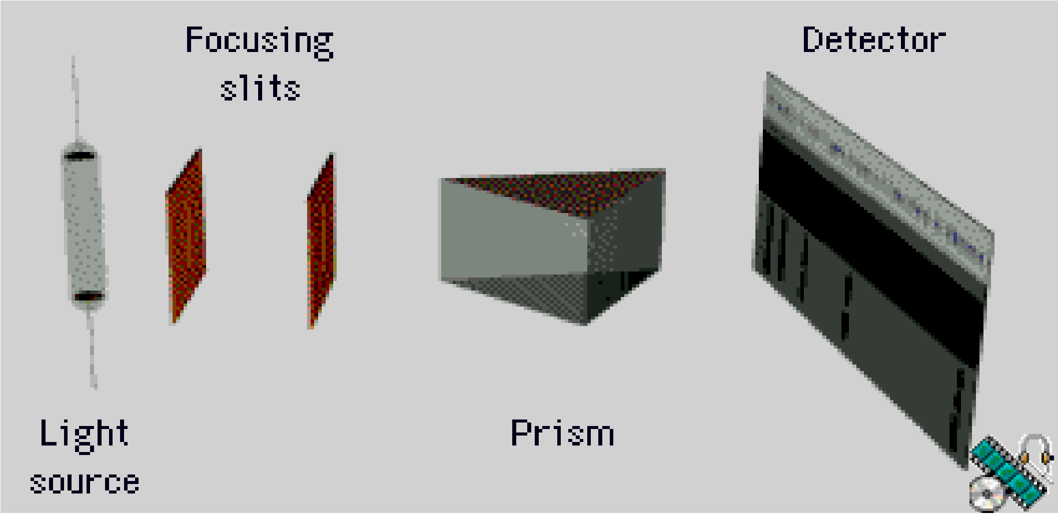
$$\text{E} = 3.83 \times 10^{-19} \text{ J per photon}$$

$$\text{For } 1.00 \text{ mol of photons:}$$

$$(6.022 \times 10^{23} \text{ photons})(3.83 \times 10^{-19} \text{ J per photon}) = 231 \text{ kJ/mol}$$

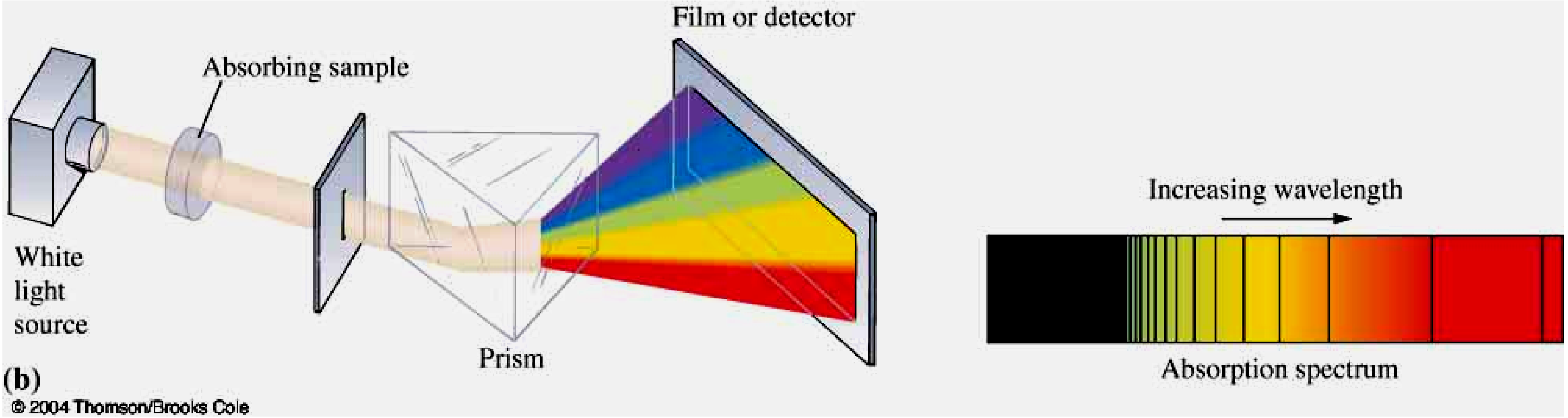
Atomic Spectra and the Bohr Atom

- An ***emission spectrum*** **is formed by an electric current passing through a gas in a vacuum tube (at very low pressure) which causes the gas to emit light.**
  - **Sometimes called a *bright* line spectrum.**



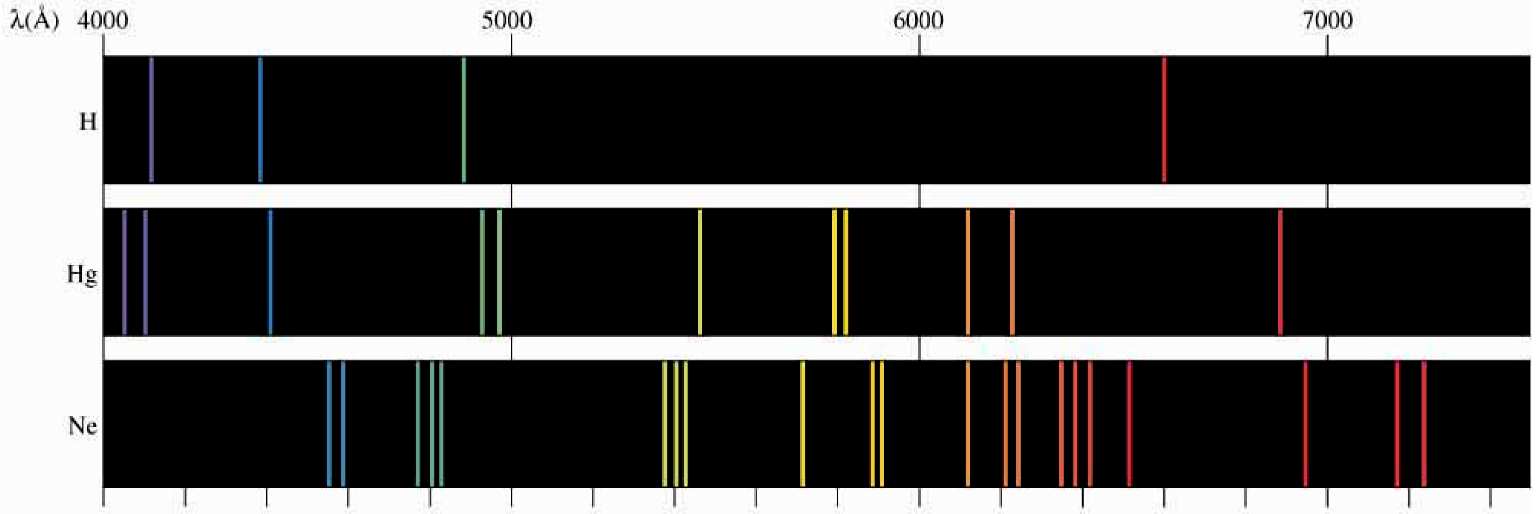
Atomic Spectra and the Bohr Atom

- An ***absorption spectrum*** **is formed by shining a beam of white light through a sample of gas.**
  - **Absorption spectra indicate the wavelengths of light that have been *absorbed*.**



Atomic Spectra and the Bohr Atom

- Every element has a unique spectrum. The spectra serves as "fingerprints"
- Thus we can use spectra to identify elements.
  - This can be done in the lab, stars, fireworks, etc.



(a)

Atomic Spectra and the Bohr Atom

- **Example: An orange line of wavelength 5890 Å is observed in the emission spectrum of sodium. What is the energy of one photon of this orange light?**

You do it!

$$\lambda = 5890 \text{ Å} \left(\frac{1 \times 10^{-10} \text{ m}}{\text{Å}} \right) = 5.890 \times 10^{-7} \text{ m}$$

$$E = h\nu = \frac{hc}{\lambda}$$

$$= \frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^{8} \text{ m/s})}{5.890 \times 10^{-7} \text{ m}}$$

$$= 3.375 \times 10^{-19} \text{ J}$$

Atomic Spectra and the Bohr Atom

- **The** **Johannes Rydberg** **equation is an empirical equation that relates the wavelengths of the lines in the hydrogen spectrum.**

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

R is the Rydberg constant

$$R = 1.097 \times 10^7 \ m^{-1}$$

$$n_1 < n_2$$

n's refer to the numbers of the energy levels in the emission spectrum of hydrogen

Johannes Rydberg

Atomic Spectra and the Bohr Atom

- **Example:** **What is the wavelength of light emitted when the hydrogen atom's energy changes from n = 4 to n = 2?**

$$n_2 = 4 \text{ and } n_1 = 2$$

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\frac{1}{\lambda} = 1.097 \times 10^7 \text{ m}^{-1}\left(\frac{1}{2^2} - \frac{1}{4^2}\right)$$

$$\frac{1}{\lambda} = 1.097 \times 10^7 \text{ m}^{-1}\left(\frac{1}{4} - \frac{1}{16}\right)$$

Atomic Spectra and the Bohr Atom

- **Example:** **What is the wavelength of light emitted when the hydrogen atom's energy changes from n = 4 to n = 2?**

$$\frac{1}{\lambda} = 1.097 \times 10^{7}\ \text{m}^{-1}\left(0.250 - 0.0625\right)$$

$$\frac{1}{\lambda} = 1.097 \times 10^{7}\ \text{m}^{-1}\left(0.1875\right)$$

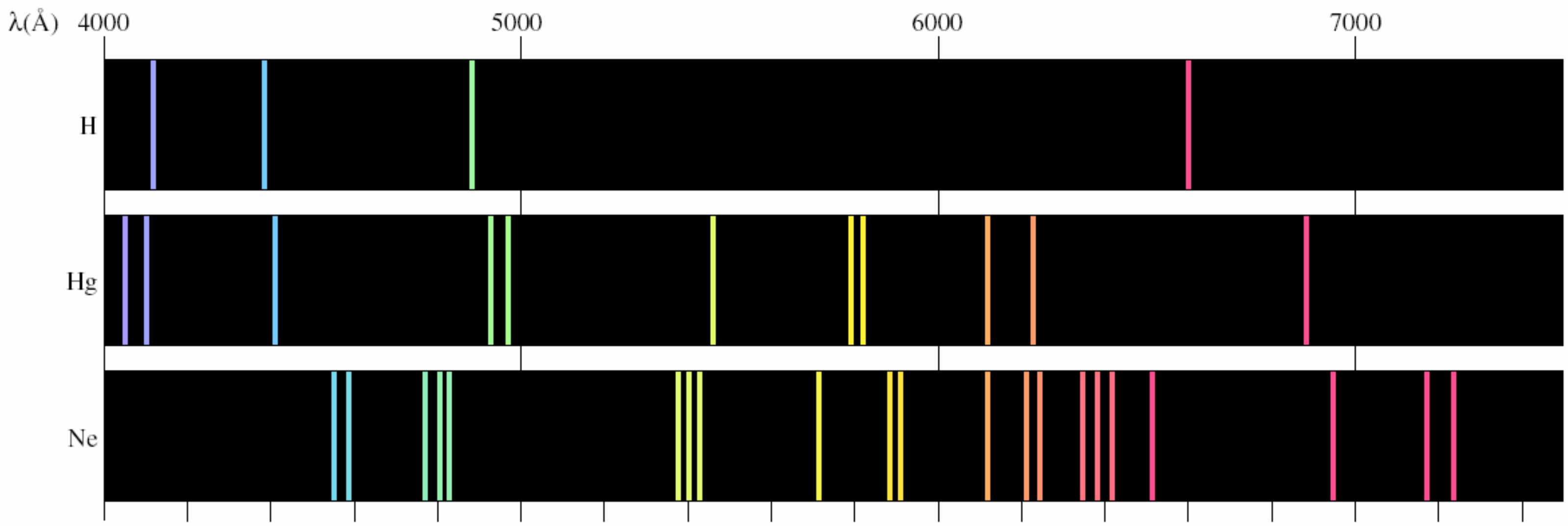
$$\frac{1}{\lambda} = 2.057 \times 10^{6}\ \text{m}^{-1}$$

$$\lambda = 4.862 \times 10^{-7}\ \text{m}$$

Atomic Spectra and the Bohr Atom

Notice that the wavelength calculated from the Rydberg equation matches the wavelength of the green colored line in the H spectrum.

$$\lambda = 4.862 \times 10^{-7}\ \text{m} = 4862\ \text{x}\ 10^{-10}\ \text{m}$$



Atomic Spectra and the Bohr Atom

- In 1913 Neils Bohr incorporated Planck's quantum theory into the hydrogen spectrum explanation. He wrote equations that described the electron of a hydrogen atom as revolving around its nucleus in circular orbits.

Neils Bohr
(Nobel prize 1922)

Atomic Spectra and the Bohr Atom

- **Here are the postulates of Bohr's theory:**

1. **Atom has a number of definite and discrete energy levels (orbits) in which an electron may exist without emitting or absorbing electromagnetic radiation.**

    As the orbital radius increases so does the energy

    1<2<3<4<5......

Atomic Spectra and the Bohr Atom

2. **An electron may move from one discrete energy level (orbit) to another, but, in so doing, monochromatic radiation is emitted or absorbed in accordance with the following equation.**

$$E_2 - E_1 = \Delta E = h\nu = \frac{hc}{\lambda}$$

$$E_2 > E_1$$

Energy is absorbed when electrons jump to higher orbits.

n = 2 to n = 4 for example

Energy is emitted when electrons fall to lower orbits.

n = 4 to n = 1 for example

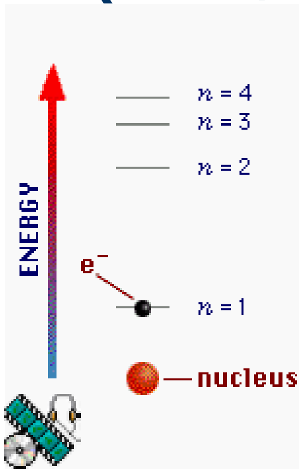
Atomic Spectra and the Bohr Atom

3. **An electron moves in a circular orbit about the nucleus and it motion is governed by the ordinary laws of mechanics and electrostatics, with the restriction that the angular momentum of the electron is quantized (can only have certain discrete values).**

Atomic Spectra and the Bohr Atom

- **Light of a characteristic wavelength (and frequency) is emitted when electrons move from higher E (orbit, n = 4) to lower E (orbit, n = 1).**
  - **This is the origin of emission spectra.**

- **Light of a characteristic wavelength (and frequency) is absorbed when electron jumps from lower E (orbit, n = 2) to higher E (orbit, n= 4)**
  - **This is the origin of absorption spectra.**



Atomic Spectra and the Bohr Atom

- Bohr's theory correctly explains the H emission spectrum.
- The theory fails for all other elements because it is not an adequate theory.

The Quantum Mechanical Picture of the Atom

- **Louis de Broglie** (1924) proposed that all moving objects have wave properties

L. de Broglie
(1892-1924)

For light: $E = mc^2$

$E = h\nu = hc / \lambda$

Therefore, $mc = h / \lambda$

and for particles (electron for example):

$(\text{mass})(\text{velocity}) = h / \lambda$

$mv = h / \lambda$

The Wave Nature of the Electron

- De Broglie's assertion was verified by **Davisson & Germer** within two years.
- Consequently, we now know that **electrons** (in fact - all particles) have both a **particle and a wave like character.**
  - This wave-particle duality is a fundamental property of submicroscopic particles.

The Wave Nature of the Electron

- **Example:** Determine the wavelength, in m, of an electron, with mass 9.11 x 10^{-31} kg, having a velocity of 5.65 x 10^{7} m/s.
  - Remember Planck's constant is 6.626 x 10^{-34} Js which is also equal to 6.626 x 10^{-34} kg m^2/s^2.

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.626\times10^{-34}\ \text{kg m}^2\cdot\text{s}^2}{\left(9.11\times10^{-31}\ \text{kg}\right)\left(5.65\times10^{7}\ \text{m/s}\right)}$$

$$\lambda = 1.29\times10^{-11}\ \text{m}$$

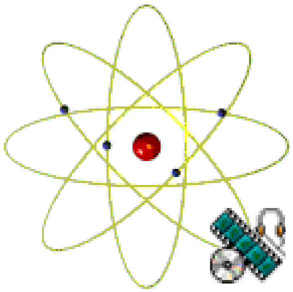
The Quantum Mechanical Picture of the Atom

W. Heisenberg
1901 - 1976

- **Werner Heisenberg in 1927 developed the concept of the Uncertainty Principle.**
- ***It is impossible to determine simultaneously both the position and momentum (mv) of an electron (or any other small particle).***
- **We define electron energy exactly but accept limitation that we do not know exact position (electron are small and move rapidly).**

The Quantum Mechanical Picture of the Atom

- Consequently, we must must speak of the **electrons' position** about the atom in terms of **probability functions**.
- These **probability functions** are represented as **orbitals** in quantum mechanics.&&&&&



The Quantum Mechanical Picture of the Atom

Basic Postulates of Quantum Theory

1. **Atoms and molecules can exist only in certain energy states.** **In each energy state, the atom or molecule has a definite energy. When an atom or molecule changes its energy state, it must emit or absorb just enough energy to bring it to the new energy state (the quantum condition).**

The Quantum Mechanical Picture of the Atom

2. **Atoms or molecules emit or absorb radiation (light), as they change their energies. The frequency of the light emitted or absorbed is related to the energy change by a simple equation.**

$$\Delta E = h\nu = \frac{hc}{\lambda}$$

The Quantum Mechanical Picture of the Atom

3. The allowed energy states of atoms and molecules can be described by sets of numbers called **quantum numbers**.

The Quantum Numbers

E. Schrodinger (1887-1961)

- **Schrodinger developed the WAVE EQUATION**
- **Solution gives set of math expressions called WAVE FUNCTIONS, ψ**
- **Each ψ describes an allowed energy state of an electron**
- **ψ is a function of distance and two angles**
- **Each ψ corresponds to an ORBITAL**

  - The region of space within which an electron is found
- **ψ does NOT describe the exact location of the electron**
- **ψ^2 is proportional to the probability of finding an electron at a given point**

The Quantum Numbers

- **Quantum numbers are the solutions of the Schrodinger, Heisenberg & Dirac equations.**
- **We use quantum numbers to designate the electronic arrangements in all atoms.**
- **Four quantum numbers (n, ℓ, m_ℓ, m_s) are necessary to describe energy states of electrons in atoms.**

$$\text{Schr}\ddot{\text{o}}\text{dinger equation (wave equation)}$$

$$-\frac{b^2}{8\pi^2 m}\left(\frac{\partial^2\Psi}{\partial^2 x}+\frac{\partial^2\Psi}{\partial^2 y}+\frac{\partial^2\Psi}{\partial^2 z}\right)+V\Psi=E\Psi$$

Quantum Numbers

- The principal quantum number has the symbol – n.

  n = 1, 2, 3, 4, ... "shells"

  n = K, L, M, N, ...

  The electron's energy depends principally on n .

Quantum Numbers

- **The angular momentum quantum number has the symbol ℓ.**

  ℓ = 0, 1, 2, 3, 4, 5, ...(n-1)

  ℓ = s, p, d, f, g, h, ...(n-1)

- **ℓ tells us the shape of the orbitals.**
- **These orbitals are the volume around the atom that the electrons occupy 90-95% of the time.**

Quantum Numbers

- The symbol for the **magnetic quantum number** is m_ℓ.

$m_\ell = -\ell, (-\ell + 1), (-\ell + 2), ...0, ..., (\ell - 2), (\ell - 1), \ell$

- If $\ell = 0$ (or an s orbital), then $m_\ell = 0$.
  - Notice that there is only 1 value of m_ℓ.

  This implies that there is one s orbital per n value. $n \geq 1$

- If $\ell = 1$ (or a p orbital), then $m_\ell = -1,0,+1$.
  - There are 3 values of m_ℓ.

  Thus there are three p orbitals per n value. $n \geq 2$

Quantum Numbers

- If $\ell = 2$ (or a d orbital), then $m_\ell = -2,-1,0,+1,+2$.
  – There are 5 values of m_ℓ.

    Thus there are five d orbitals per n value. $n \geq 3$

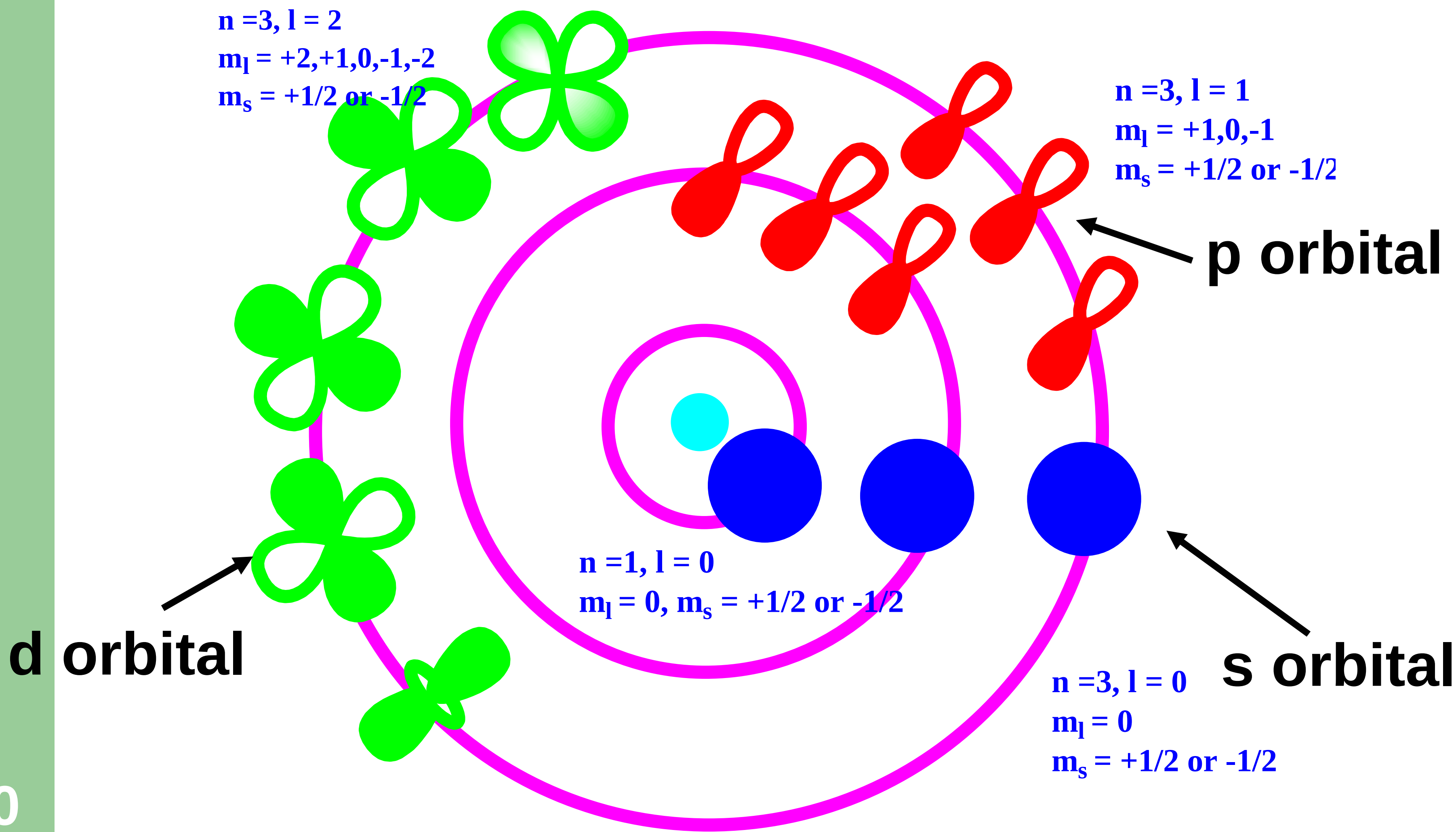
- If $\ell = 3$ (or an f orbital), then $m_\ell = -3,-2,-1,0,+1,+2, +3$.
  – There are 7 values of m_ℓ.

    Thus there are seven f orbitals per n value, n

Quantum Numbers

- The last quantum number is the spin quantum number which has the symbol m_s.
- The spin quantum number only has two possible values.
  - $m_s = +1/2$ or $-1/2$
  - $m_s = \pm 1/2$
- This quantum number tells us the spin and orientation of the magnetic field of the electrons.
- Wolfgang Pauli in 1925 discovered the Exclusion Principle.
  - No two electrons in an atom can have the same set of 4 quantum numbers.

Quantum Numbers



Atomic Orbitals

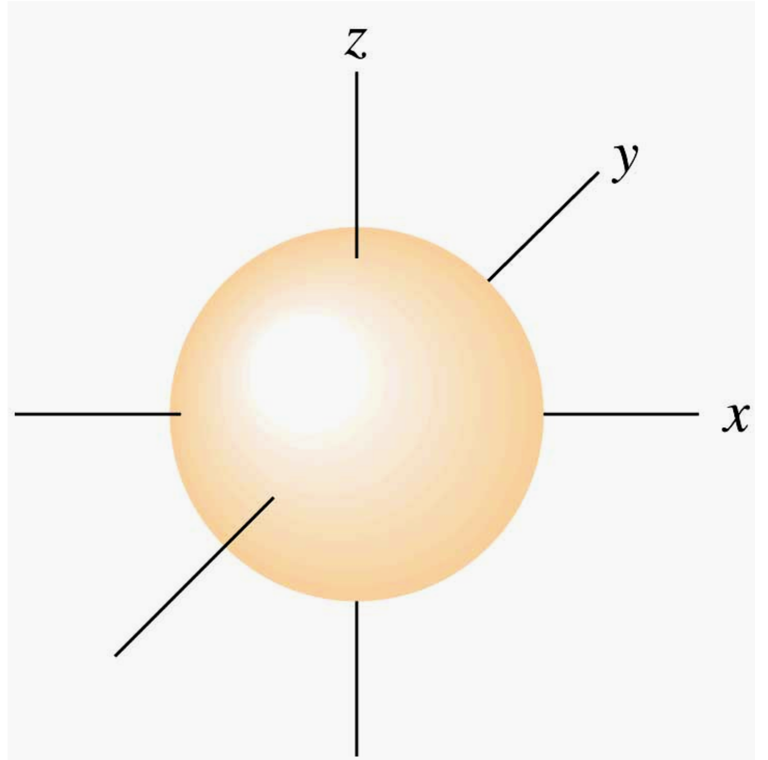
- **Atomic orbitals** are regions of space where the probability of finding an electron about an atom is highest.
- **s orbital** properties:

  - s orbitals are spherically symmetric.

  – There is one s orbital per n level.

  – $\ell = 0$

  – 1 value of m_ℓ

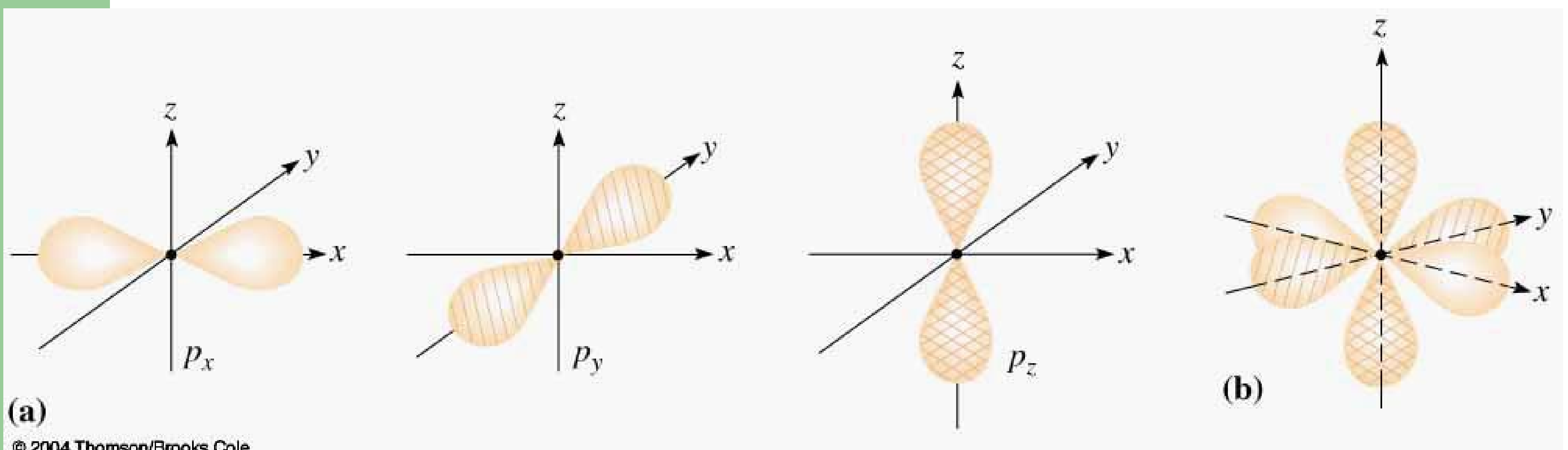


Atomic Orbitals

- p orbital properties:
  - The first p orbitals appear in the n = 2 shell.
- p orbitals are peanut or dumbbell shaped volumes.
  - They are directed along the axes of a Cartesian coordinate system.
- There are 3 p orbitals per n level.
  - The three orbitals are named p_x, p_y, p_z.
  - They have an $\ell = 1$.
  - $m_\ell = -1,0,+1$ 3 values of m_ℓ

Atomic Orbitals

- p orbitals are peanut or dumbbell shaped.

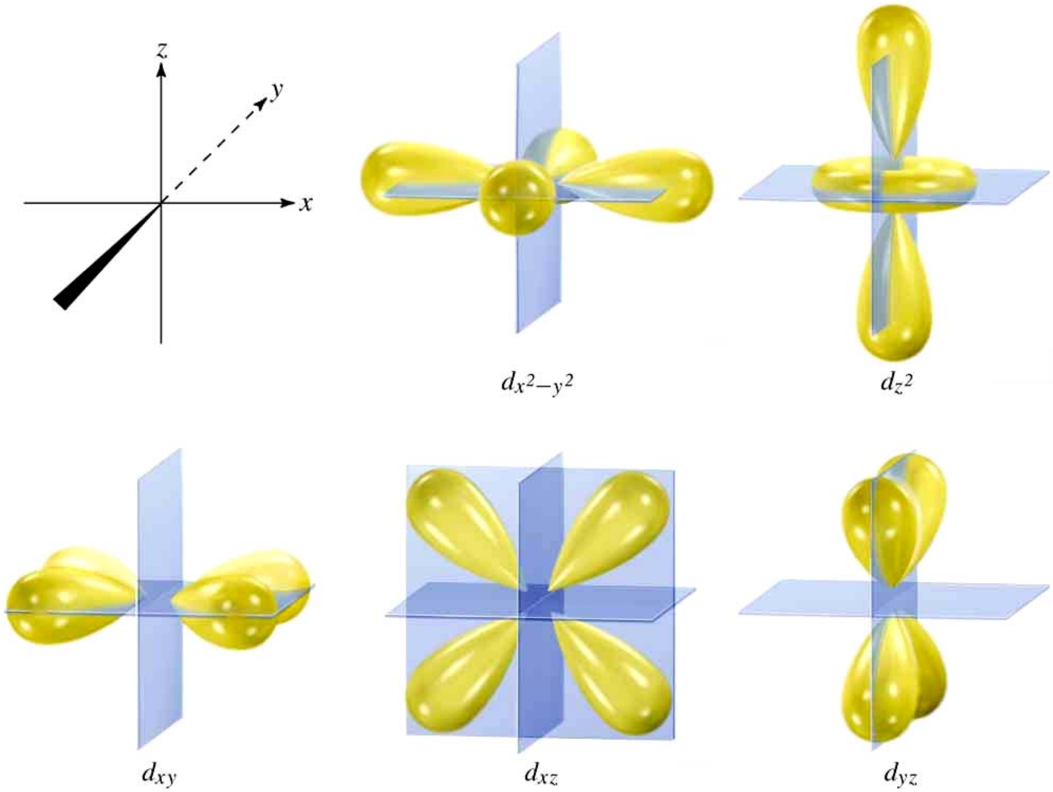


Atomic Orbitals

- d orbital properties:
  - The first d orbitals appear in the n = 3 shell.
- The five d orbitals have two different shapes:
  - 4 are clover leaf shaped.
  - 1 is peanut shaped with a doughnut around it.
  - The orbitals lie directly on the Cartesian axes or are rotated 45° from the axes.
- There are 5 d orbitals per n level.
  - The five orbitals are named $d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$
  - They have an $\ell = 2$.
  - m_ℓ = -2,-1,0,+1,+2 5 values of m_ℓ

Atomic Orbitals

- d orbital shapes



Atomic Orbitals

- f orbital properties:
  - The first f orbitals appear in the n = 4 shell.
- The f orbitals have the most complex shapes.
- There are seven f orbitals per n level.
  - The f orbitals have complicated names.
  - They have an $\ell = 3$
  - m_ℓ = -3,-2,-1,0,+1,+2, +3   7 values of m_ℓ
  - The f orbitals have important effects in the lanthanide and actinide elements.

Atomic Orbitals

- f orbital properties:
  - <u>The first f orbitals appear in the n = 4 shell.</u>
- The f orbitals have the most complex shapes.
- There are seven f orbitals per n level.
  - The f orbitals have complicated names.
  - They have an $\ell = 3$
  - m_ℓ = -3,-2,-1,0,+1,+2, +3   7 values of m_ℓ
  - The f orbitals have important effects in the lanthanide and actinide elements.

Atomic Orbitals

- **Spin quantum number effects:**
  - Every orbital can hold up to two electrons.
    - Consequence of the Pauli Exclusion Principle.
  - The two electrons are designated as having
  - one spin up ↑ and one spin down ↓
- Spin describes the direction of the electron's magnetic fields.

Paramagnetism and Diamagnetism

- Atoms with unpaired $\underline{\uparrow\uparrow}$ electrons are called ***paramagnetic***.
  - Paramagnetic atoms are attracted to a magnet.

- Atoms with paired $\underline{\uparrow\downarrow}$ electrons are called ***diamagnetic***.
  - Diamagnetic atoms are repelled by a magnet.

Paramagnetism and Diamagnetism

- **Because two electrons in the same orbital must be paired, it is possible to calculate the number of orbitals and the number of electrons in each n shell.**
- **The number of orbitals per n level is given by n^2.**
- **The maximum number of electrons per n level is $2n^2$.**

Paramagnetism and Diamagnetism

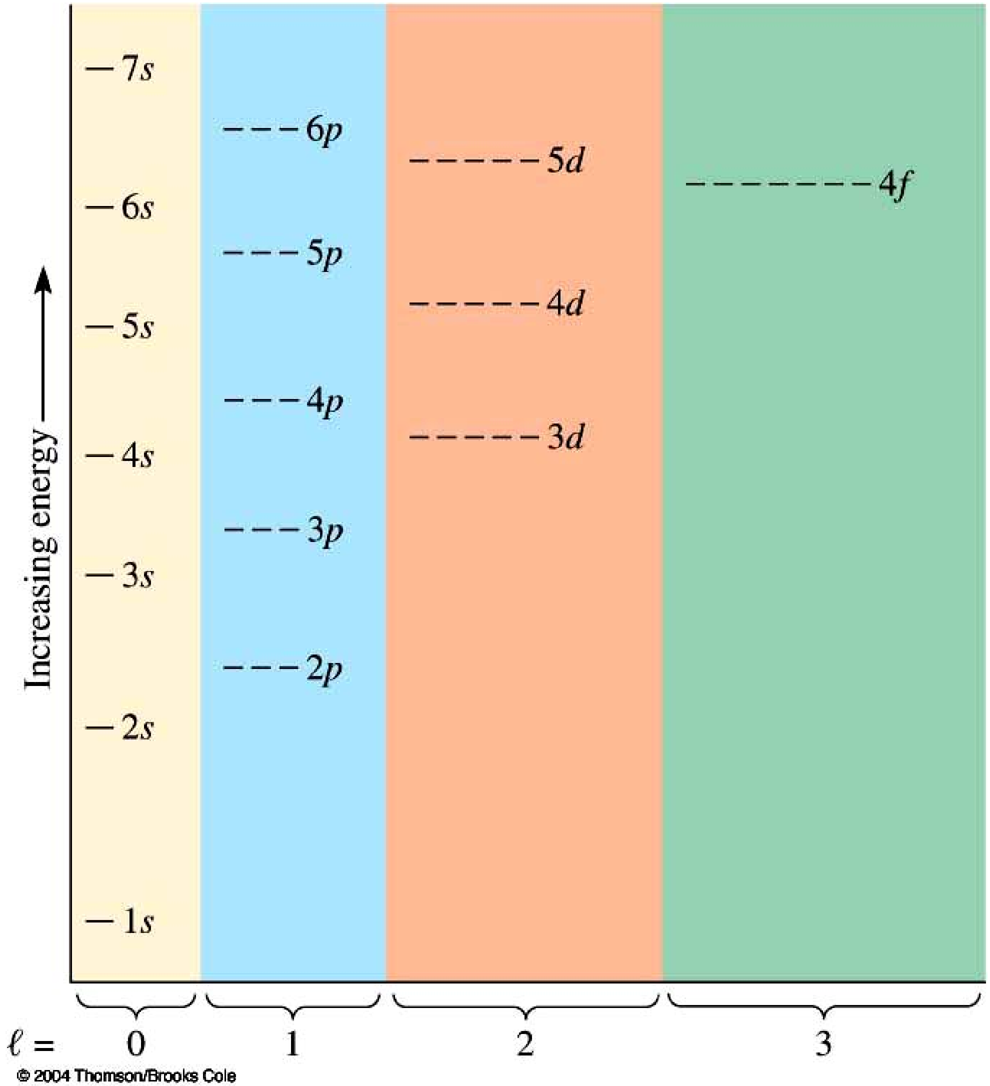
Energy Level	# of Orbitals	Max. # of e^-
n	n^2	$2n^2$
1	1	2
2	4	8
3	9	18
4	16	32

The Periodic Table and Electron Configurations

- The principle that describes how the periodic chart is a function of electronic configurations is the **Aufbau Principle**.
- The electron that distinguishes an element from the previous element enters the lowest energy atomic orbital available.

The Periodic Table and Electron Configurations

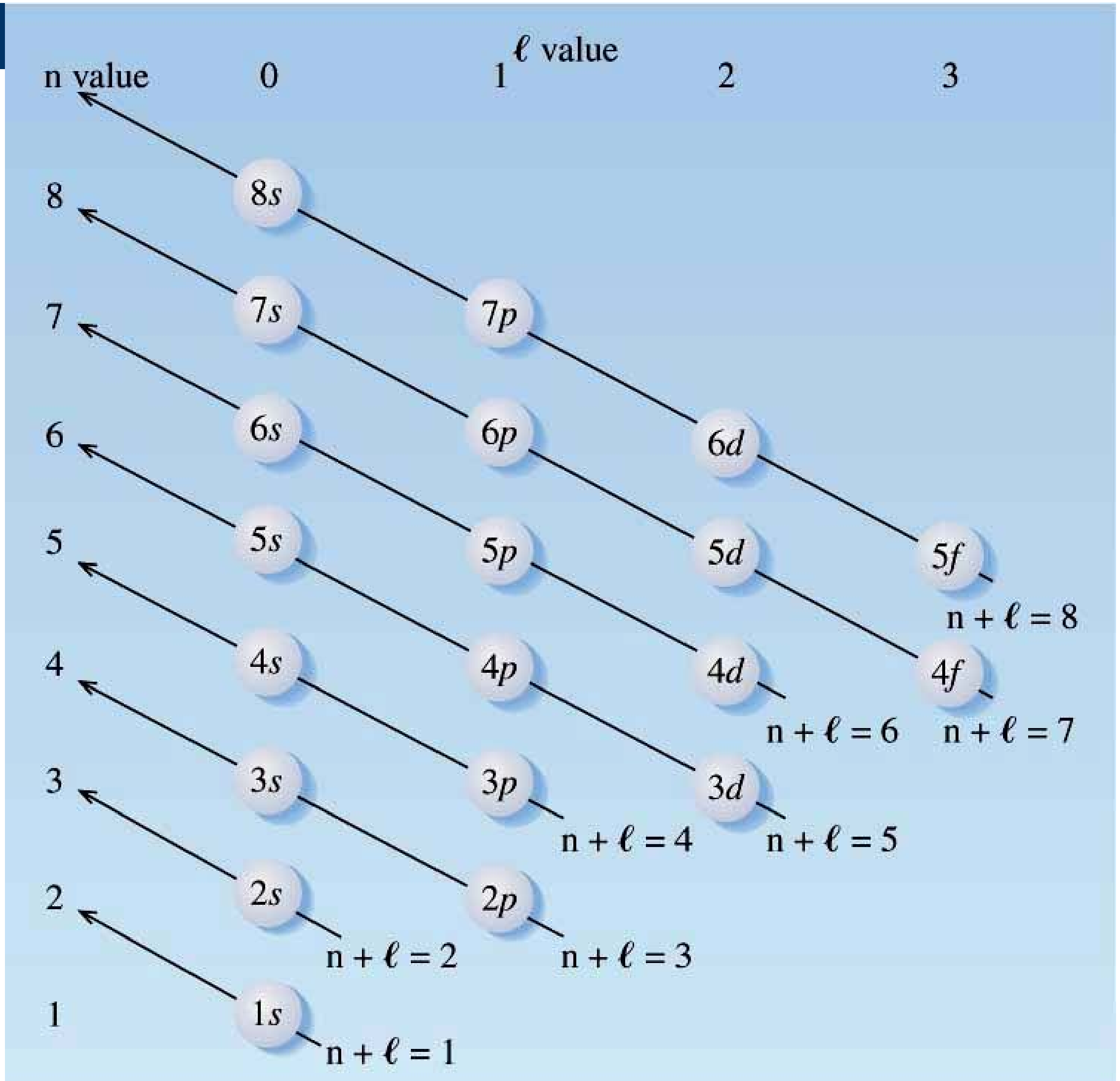
- **The Aufbau Principle describes the electron filling order in atoms.**



The Periodic Table and Electron Configurations

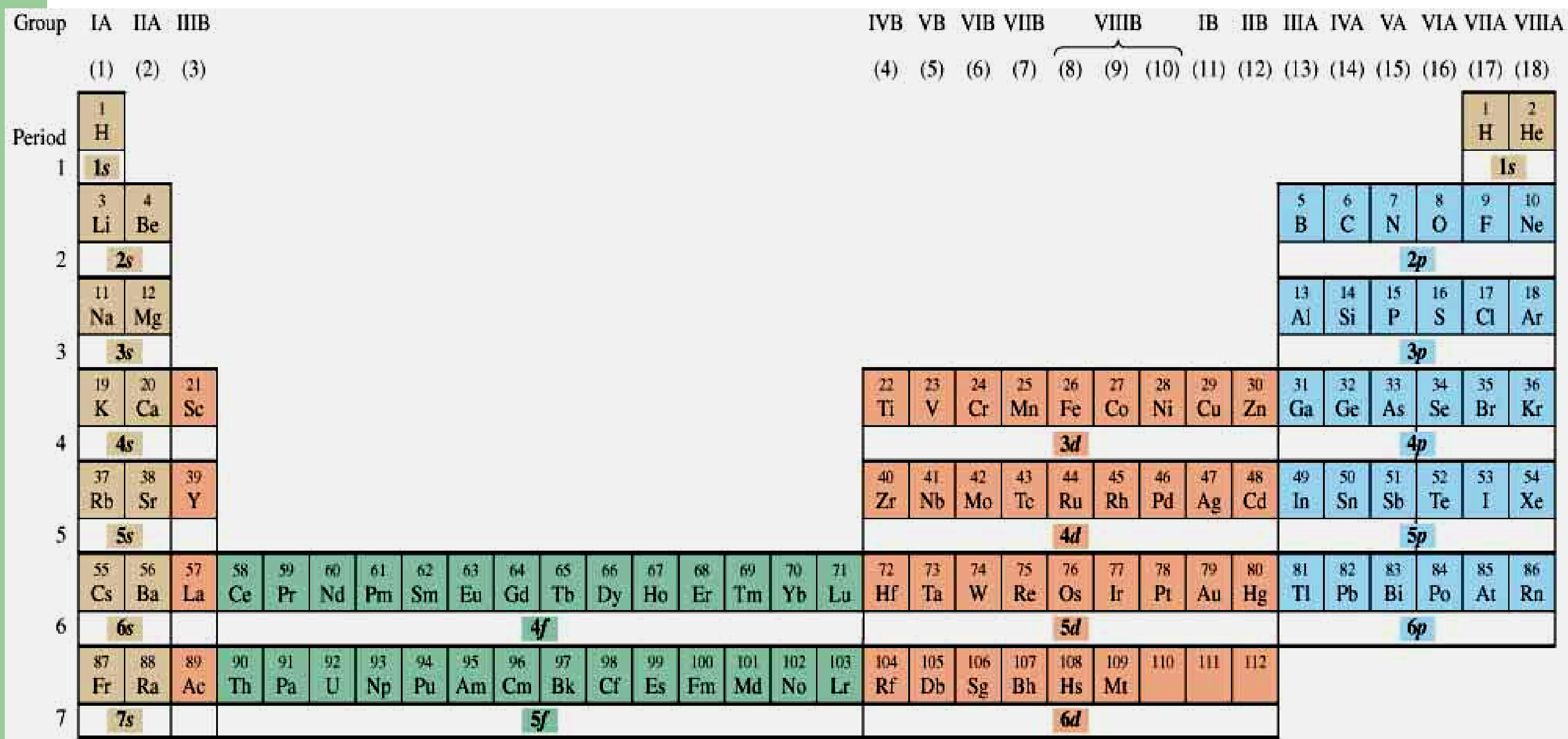
- There are two ways to remember the correct filling order for electrons in atoms.

1. You can use this mnemonic.



The Periodic Table and Electron Configurations

2. **Or you can use the periodic chart .**



Hund's rule

- **<u>Hund's rule</u> tells us that the electrons will fill the p orbitals by placing electrons in each orbital singly and with same spin until half-filled. Then the electrons will pair to finish the p orbitals.**

The Periodic Table and Electron Configurations

- **1st row elements**

	1s	Configuration
$_1H$	↑	$1s^1$

	1s	Configuration
$_1H$	↑	$1s^1$
$_2He$	↑↓	$1s^2$

The Periodic Table and Electron Configurations

- **2nd row elements**

	1s	2s	2p	Configuration
$_3$Li	↑↓	↑	_ _ _	$1s^2\ 2s^1$
$_4$Be	↑↓	_	_ _ _	$1s^2\ 2s^2$
$_5$B	↑↓	↑↓	↑ _ _	$1s^2\ 2s^2\ 2p^1$
$_6$C	↑↓	↑↓	↑ ↑ _	$1s^2\ 2s^2\ 2p^2$
$_7$N	↑↓	↑↓	_ _ _	$1s^2\ 2s^2\ 2p^3$
$_8$O	↑↓	↑↓	↑↓ ↑ ↑	$1s^2\ 2s^2\ 2p^4$
$_9$F	↑↓	↑↓	↑↓ ↑↓ ↑	$1s^2\ 2s^2\ 2p^5$
$_{10}$Ne	↑↓	↑↓	↑↓ ↑↓ ↑↓	$1s^2\ 2s^2\ 2p^6$

The Periodic Table and Electron Configurations

- **3rd row elements**

		3s	3p			Configuration
$_{11}$Na	[Ne]	↑	_	_	_	$[Ne]3s^1$
$_{12}$Mg	[Ne]	_	_	_	_	$[Ne]3s^2$
$_{13}$Al	[Ne]	↑↓	↑	_	_	$[Ne]3s^2\ 3p^1$
$_{14}$Si	[Ne]	↑↓	↑	↑	_	$[Ne]3s^2\ 3p^2$
$_{15}$P	[Ne]	↑↓	↑	↑	↑	$[Ne]3s^2\ 3p^3$
$_{16}$S	[Ne]	↑↓	_	_	_	$[Ne]3s^2\ 3p^4$
$_{17}$Cl	[Ne]	↑↓	↑↓	↑↓	↑	$[Ne]3s^2\ 3p^5$
$_{18}$Ar	[Ne]	↑↓	↑↓	↑↓	↑↓	$[Ne]3s^2\ 3p^6$

There is an extra measure of stability associated with half-filled or completely filled orbitals.

		3d					4s	4p			Configuration
$_{19}$K	[Ar]						↑				[Ar]$4s^1$
$_{20}$Ca	[Ar]						↑↓				[Ar]$4s^2$
$_{21}$Sc	[Ar]	↑					↑↓				[Ar]$4s^2\ 3d^1$
$_{22}$Ti	[Ar]	↑	↑				↑↓				[Ar]$4s^2\ 3d^2$
$_{23}$V	[Ar]	↑	↑	↑			↑↓				[Ar]$4s^2\ 3d^3$
$_{24}$Cr	[Ar]	↑	↑	↑	↑	↑	↑				[Ar]$4s^1\ 3d^5$

The Periodic Table and Electron Configurations

	3d					4s	4p			Configuration
$_{25}$Mn [Ar]	↑	↑	↑	↑	↑	↑↓				$[Ar]4s^2\ 3d^5$
$_{26}$Fe [Ar]	↑↓	↑	↑	↑	↑	↑↓				$[Ar]4s^2\ 3d^6$
$_{27}$Co [Ar]	↑↓	↑↓	↑	↑	↑	↑↓				$[Ar]4s^2\ 3d^7$
$_{28}$Ni [Ar]	↑↓	↑↓	↑↓	↑	↑	↑↓				$[Ar]4s^2\ 3d^8$
$_{29}$Cu [Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑				$[Ar]4s^1\ 3d^{10}$
$_{30}$Zn [Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓				$[Ar]4s^2\ 3d^{10}$

The Periodic Table and Electron Configurations

		3d					4s	4p			Configuration
$_{31}$Ga	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑			$[Ar]4s^2\ 3d^{10}\ 4p^1$
$_{32}$Ge	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑		$[Ar]4s^2\ 3d^{10}\ 4p^2$
$_{33}$As	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	$[Ar]4s^2\ 3d^{10}\ 4p^3$
$_{34}$Se	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	$[Ar]4s^2\ 3d^{10}\ 4p^4$
$_{35}$Br	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$[Ar]4s^2\ 3d^{10}\ 4p^5$
$_{36}$Kr	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	$[Ar]4s^2\ 3d^{10}\ 4p^6$

The Periodic Table and Electron Configurations

- **Now we can write a complete set of quantum numbers for all of the electrons in these three elements as examples.**
  - **Na**
  - **Ca**
  - **Fe**

	3s	3p	Configuration
$_{11}Na$ [Ne]	↑	__ __ __	$[Ne]3s^1$

	n	ℓ	m_ℓ	m_s	
1st e⁻	1	0	0	+ 1/2	1 s electrons
2nd e⁻	1	0	0	– 1/2	
3rd e⁻	2	0	0	+ 1/2	2 s electrons
4th e⁻	2	0	0	– 1/2	
5th e⁻	2	1	- 1	+ 1/2	2 p electrons
6th e⁻	2	1	0	+ 1/2	
7th e⁻	2	1	+ 1	+ 1/2	
8th e⁻	2	1	– 1	– 1/2	
9th e⁻	2	1	0	– 1/2	
10th e⁻	2	1	+ 1	– 1/2	
11th e⁻	3	0	0	+ 1/2	3 s electron

	3d	4s	4p	Configuration
$_{20}$Ca [Ar]	_ _ _ _ _	↑↓	_ _ _	$[Ar]\,4s^2$

	n	ℓ	m_ℓ	m_s	
[Ar] 19^{th} e^-	4	0	0	+1/2	4 s electrons
20^{th} e^-	4	0	0	−1/2	

	3d					4s	4p	Configuration
$_{26}Fe$ [Ar]	↑↓	↑	↑	↑	↑	↑↓	_ _ _	$[Ar]4s^2\ 3d^6$

	n	ℓ	m_ℓ	m_s	
[Ar] $19^{th}\ e^-$	4	0	0	+1/2	4 s electrons
$20^{th}\ e^-$	4	0	0	−1/2	
$21^{st}\ e^-$	3	2	-2	+1/2	
$22^{nd}\ e^-$	3	2	-1	+1/2	
$23^{rd}\ e^-$	3	2	0	+1/2	
$24^{th}\ e^-$	3	2	+1	+1/2	
$25^{th}\ e^-$	3	2	+2	+1/2	
$26^{th}\ e^-$	3	2	-2	−1/2	

Chapter 5 – The Structure of Atoms

- Fundamental particles (p, n, e) in atoms and ions
- Rutherford Experiment – Conclusions
- Atomic number (Z), mass number A $\quad {}_{Z}^{A}E$
- Atomic weight (weight average of isotopes)
- Relationship between ν, λ, E, c, h

$$C = \lambda\nu \qquad E = h\nu = hc / \lambda$$

- Bohr atom
- Rydberg equation, relationship between λ and energy levels n

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

Chapter 5 – The Structure of Atoms

- Quantum mechanics – Heisenberg Uncertainty Principle.
  - Quantum numbers (n, ℓ, m_ℓ, m_s)
  - Pauli Exclusion Principle
- Electron configuration of atoms (Hunds Rule)
  - Filling orbitals – s, p, d, f (except Cu, Cr)
  - diamagnetic *vs* paramagnetic
  - maximum # electron's in major energy level = $2n^2$
- Atomic Orbital representations (pictures)
  - s, p_x p_y p_z, d_{z^2} $d_{x^2-y^2}$ d_{xy} d_{xz} d_{yz}
- Relationship between quantum numbers, electronic configuration, and periodic table.

Homework Assignment

One-line Web Learning (OWL):

Chapter 5 Exercises and Tutors – Optional