Atomic Structure and Periodicity

Wave Partilce Duality

** Not Part of class**

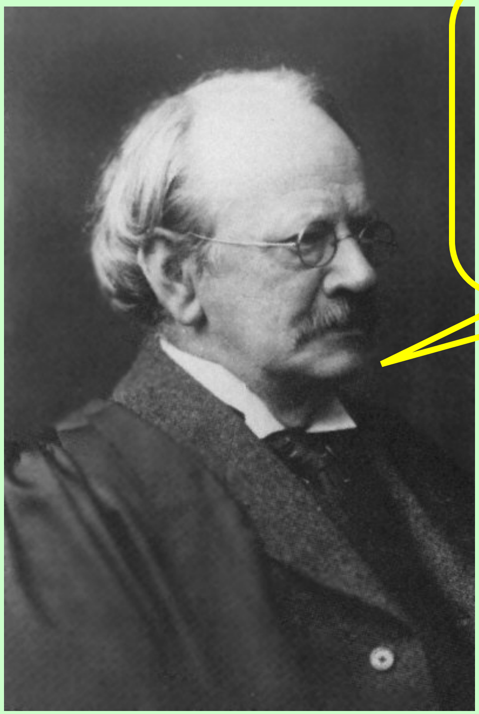
The Puzzle of the Atom

- Protons and electrons are attracted to each other because of opposite charges
- Electrically charged particles moving in a curved path give off energy
- Despite these facts, atoms don’t collapse

Wave-Particle Duality

JJ Thomson won the Nobel prize for describing the electron as a particle.

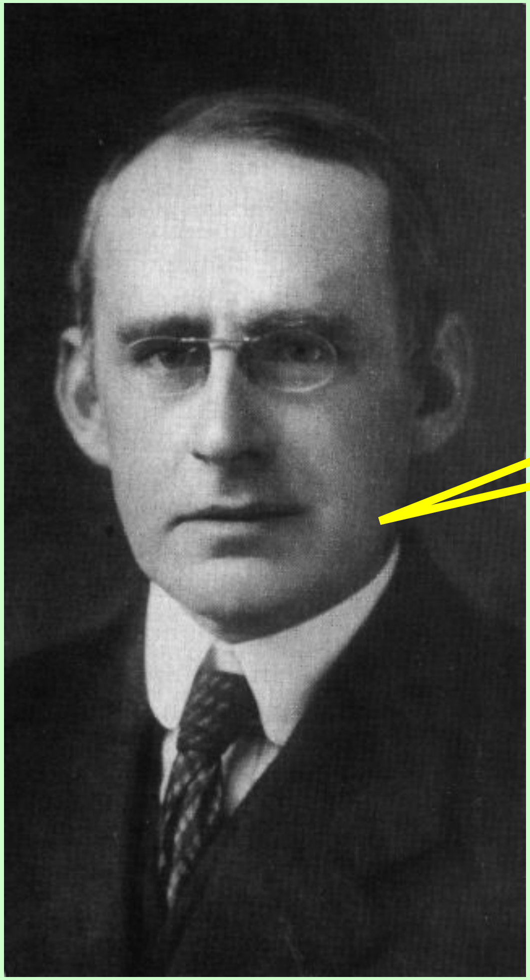
His son, George Thomson won the Nobel prize for describing the wave-like nature of the electron.



The electron is a particle!

The electron is an energy wave!

Confused??? You've Got Company!



"No familiar conceptions can be woven around the electron; something unknown is doing we don't know what."

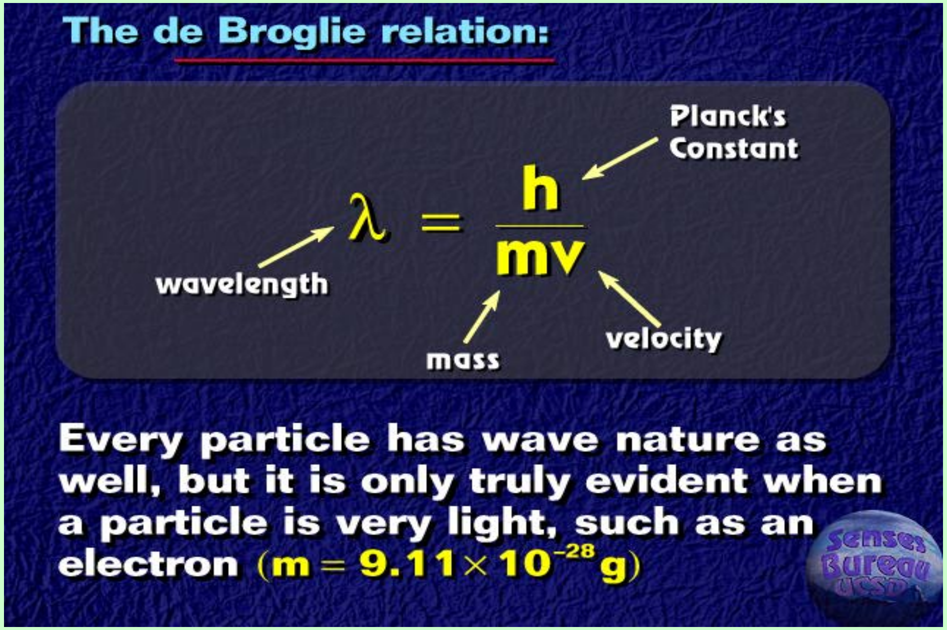
Physicist Sir Arthur Eddington

The Nature of the Physical World

1934

The Wave-like Electron

The electron propagates through space as an energy wave. To understand the atom, one must understand the behavior of electromagnetic waves.



Light Travels through space as a wave

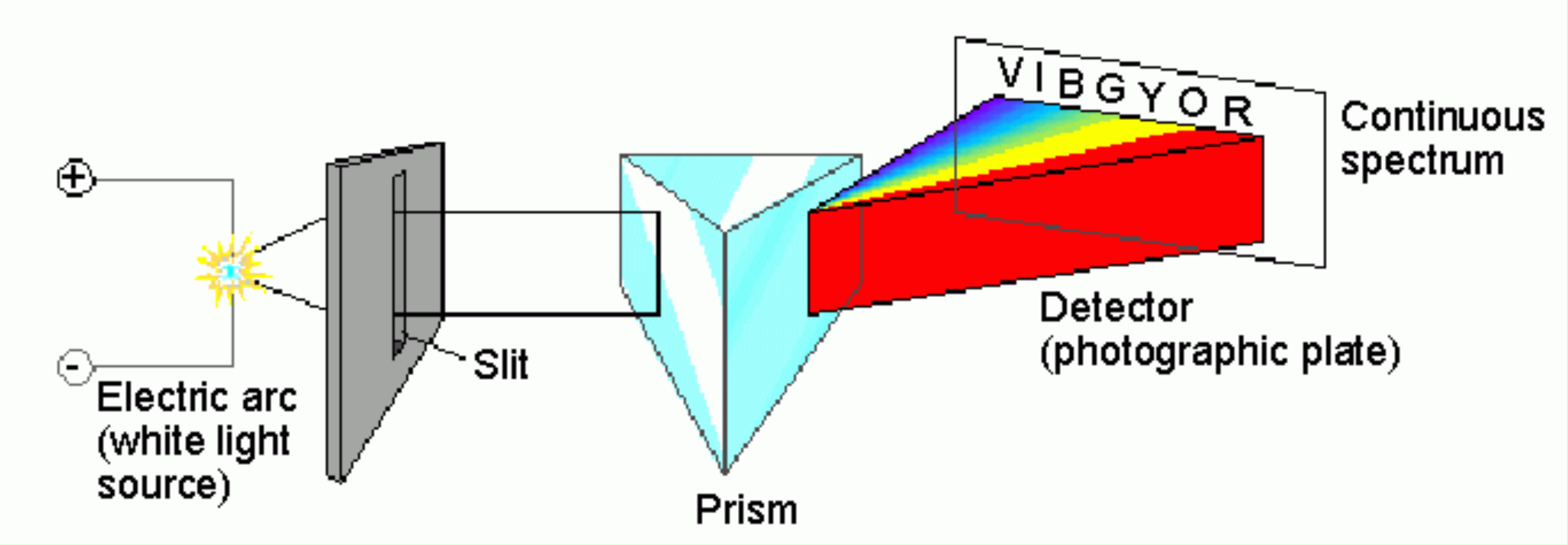
Light transmits energy as a particle

Particles have wavelength, exhibited by diffraction patterns

- Large particles have very short wavelength
- All Matter exhibits both particle and wave properties

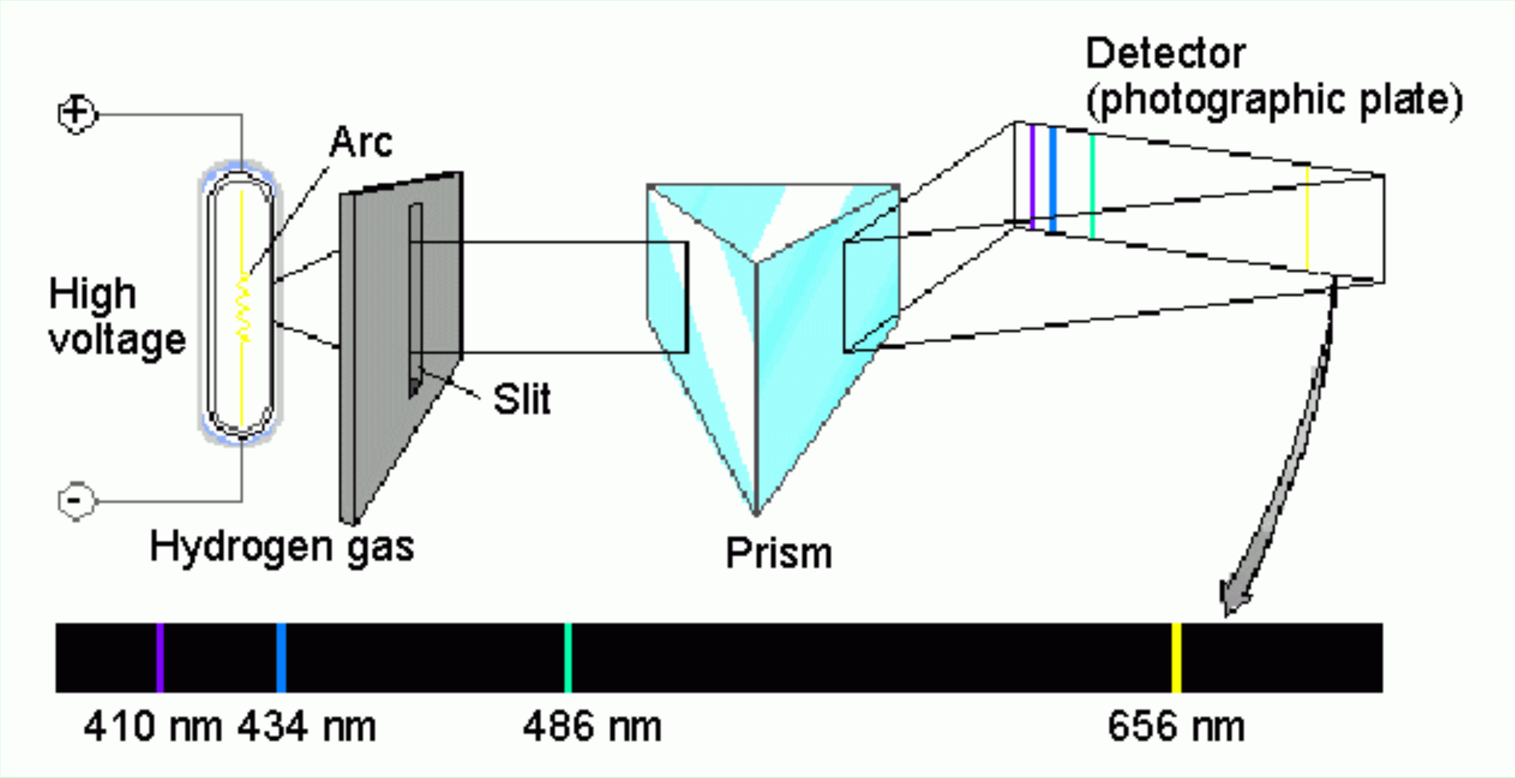
Spectroscopic analysis of the visible spectrum…

…produces all of the colors in a continuous spectrum



Spectroscopic analysis of the hydrogen spectrum…

…produces a "bright line" spectrum



Electron Energy in Hydrogen
The Bohr Model

- Bohr Model
  - The electron moves around the nucleus only in certain allowed circular orbits
  - Bright line spectra confirms that only certain energies exist in the atom, and atom emits photons with definite wavelengths when the electron returns to a lower energy state
  - Energy levels available to the electron in the hydrogen atom

Shortcomings of Bohr Model…

1. Bohr's model does not work for atoms other than hydrogen

2. Electron's do not move in circular orbits

Schrodinger Wave Equation

Erwin Schrodinger

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2}+V\psi=E\psi$$

Equation for **probability** of a single electron being found along a single axis (x-axis)

Heisenberg Uncertainty Principle

Werner Heisenberg

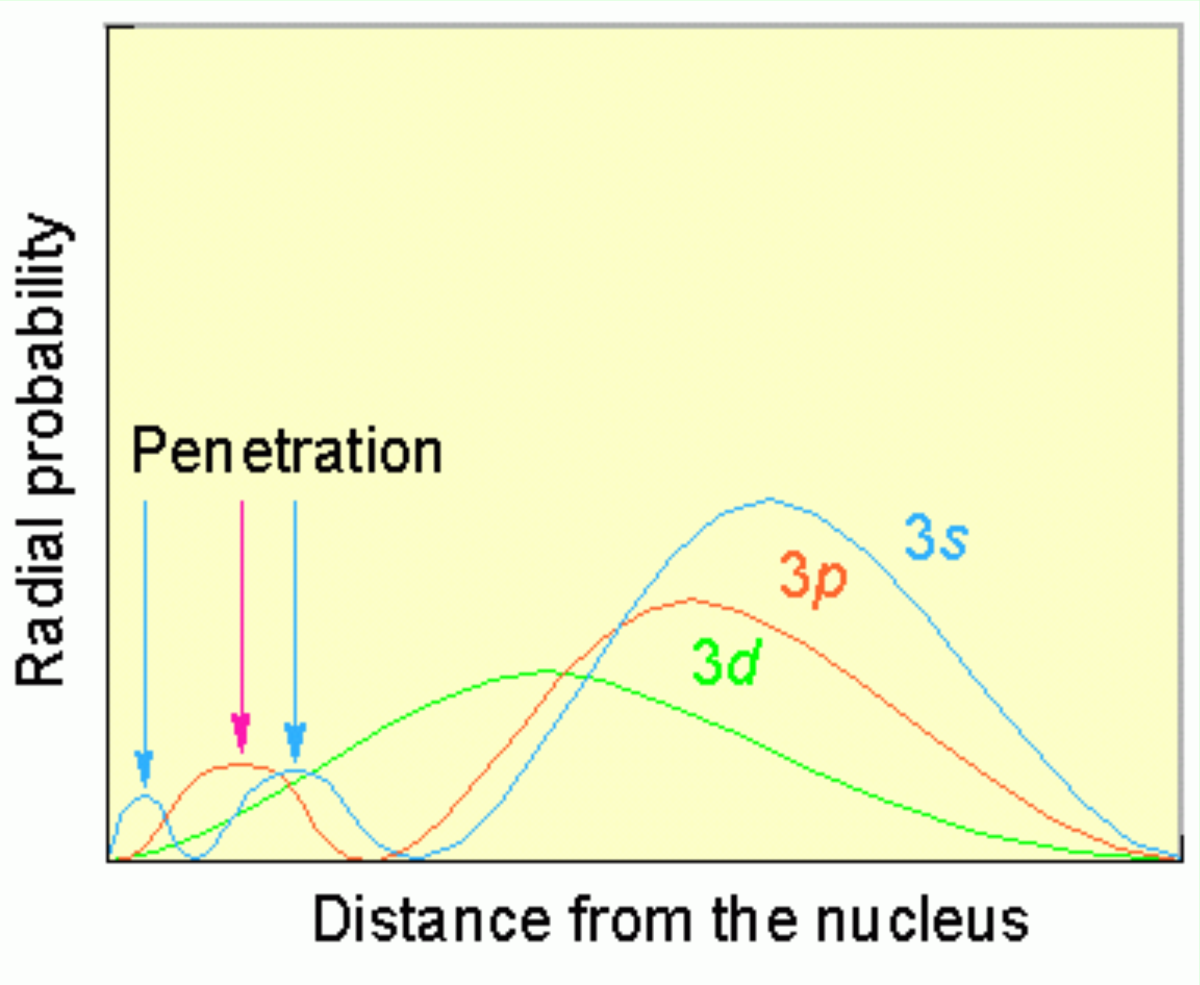
"One cannot simultaneously determine both the position and momentum of an electron."

You can find out where the electron is, but not where it is going.

OR…

You can find out where the electron is going, but not where it is!

Which of the orbital types in the 3rd energy level does not seem to have a "node"?



<u>WHY NOT?</u>

Quantum Numbers

Each electron in an atom has a unique set of 4 quantum numbers which describe it.

- Principal quantum number, n
- Angular momentum quantum number, l
- Magnetic quantum number, m or m_l
- Spin quantum number, s or m_s

Pauli Exclusion Principle

Wolfgang Pauli

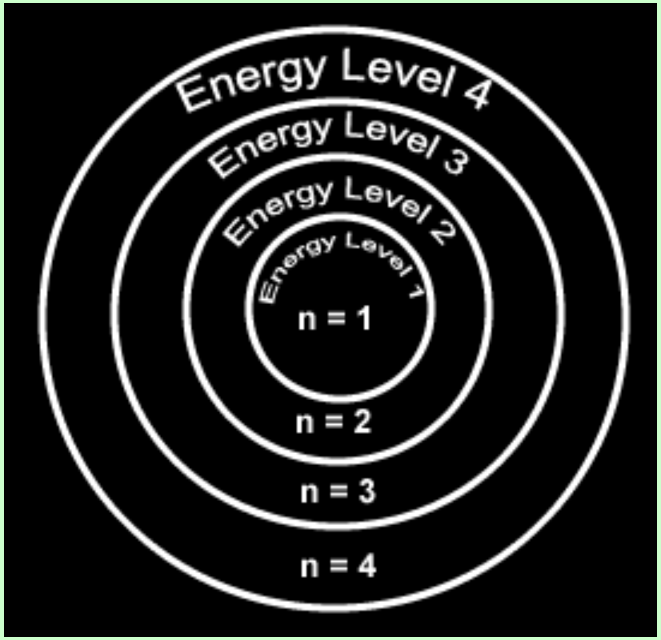
No two electrons in an atom can have the same four quantum numbers.

Principal Quantum Number

Generally symbolized by n, it denotes the shell (energy level) in which the electron is located.

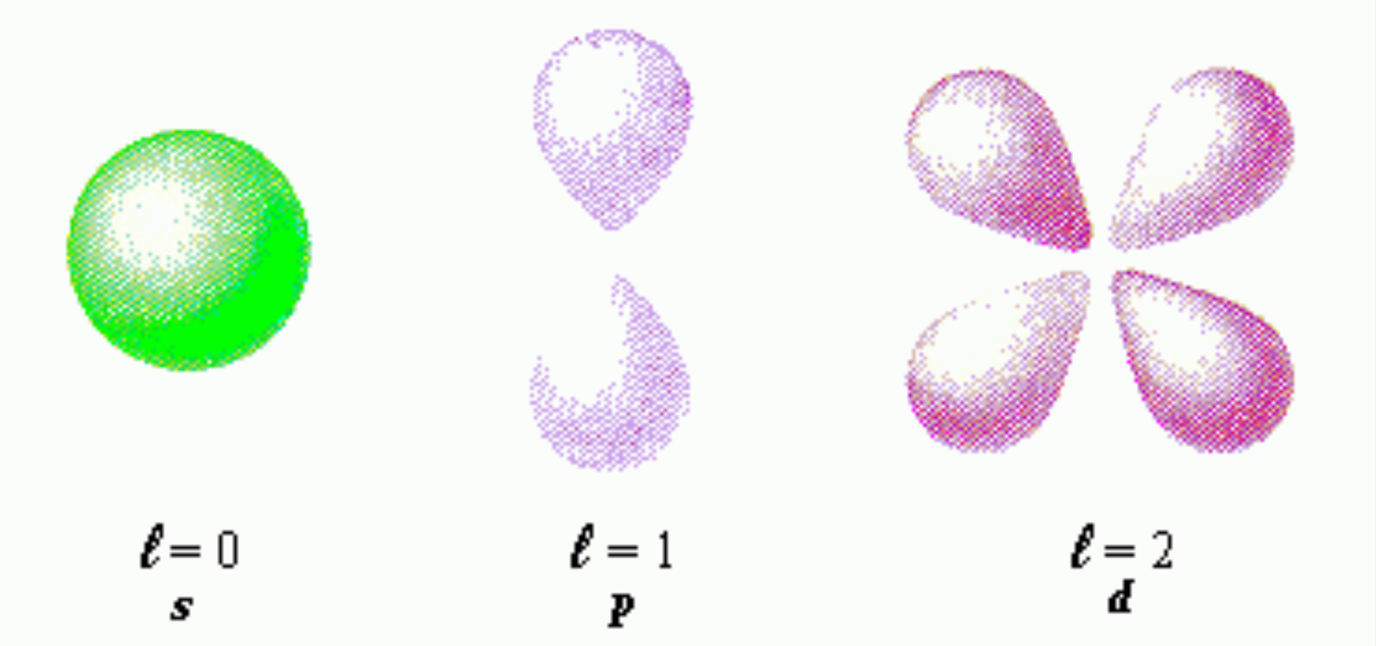
Number of electrons that can fit in a shell:

$$2n^2$$



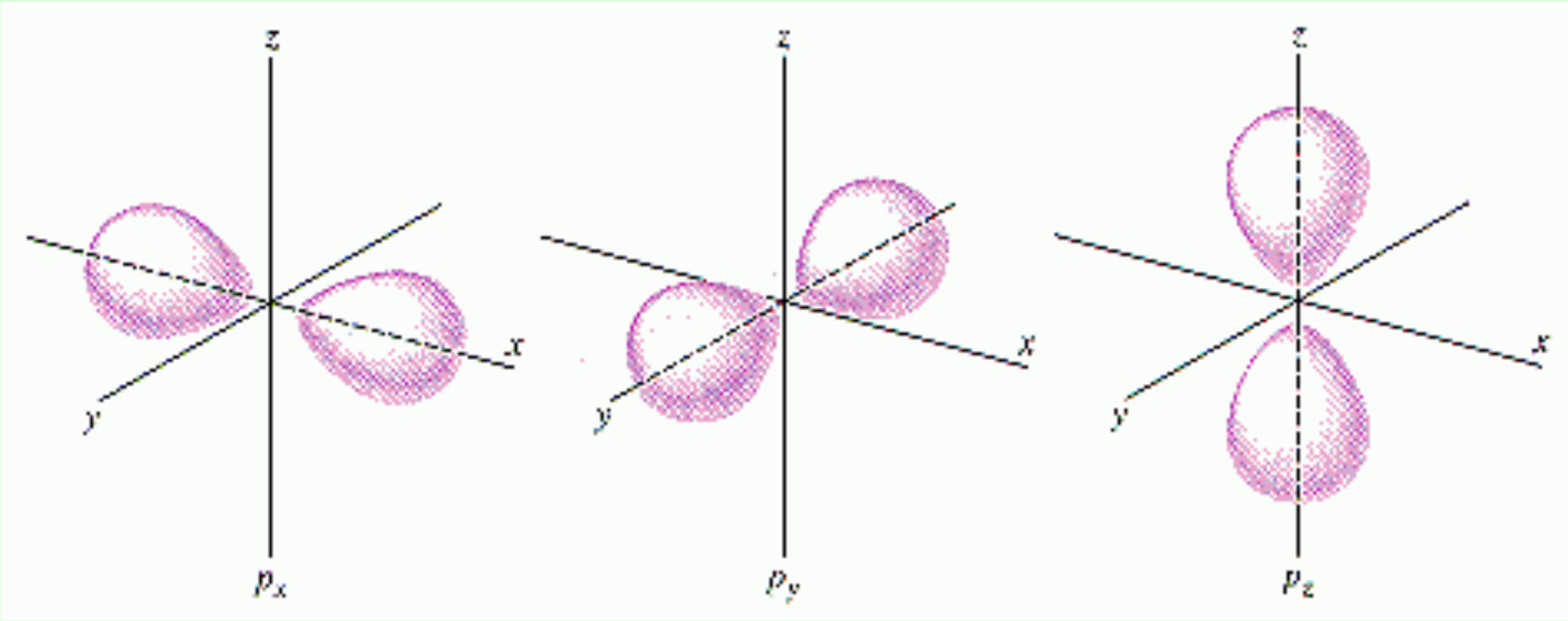
Angular Momentum Quantum Number

The angular momentum quantum number, generally symbolized by l, denotes the orbital (subshell) in which the electron is located.



Magnetic Quantum Number

The magnetic quantum number, generally symbolized by *m*, denotes the orientation of the electron's orbital with respect to the three axes in space.



Spin Quantum Number

Spin quantum number denotes the behavior (direction of spin) of an electron within a magnetic field.

Possibilities for electron spin:

$$+\frac{1}{2} \qquad -\frac{1}{2}$$

Assigning the Numbers

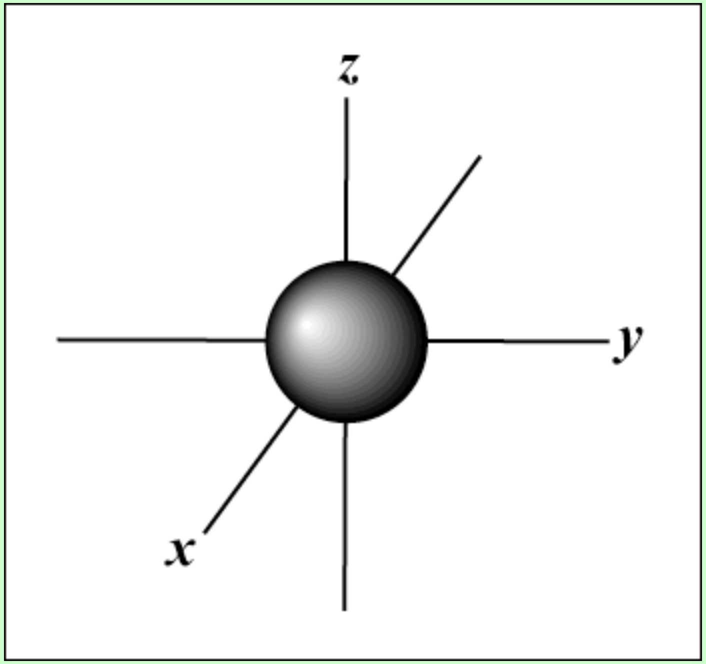
- The three quantum numbers (*n*, *l*, and *m*) are integers.
- The principal quantum number (*n*) cannot be zero.
- *n* must be 1, 2, 3, etc.
- The angular momentum quantum number (*l*) can be any integer between 0 and n - 1.
- For *n* = 3, *l* can be either 0, 1, or 2.
- The magnetic quantum number (m_l) can be any integer between -*l* and +*l*.
- For *l* = 2, *m* can be either -2, -1, 0, +1, +2.

Principle, angular momentum, and magnetic quantum numbers: *n*, *l*, and m_l

Table 7.2 Quantum numbers for the first four levels of orbitals in the hydrogen atom

n	*l*	Orbital designation	m_l	# of orbitals
1	0	1s	0	1
2	0	2s	0	1
	1	2p	-1, 0, 1	3
3	0	3s	0	1
	1	3p	-1, 0, 1	3
	2	3d	-2, -1, 0, 1, 2	5
4	0	4s	0	1
	1	4p	-1, 0, 1	3
	2	4d	-2, -1, 0, 1, 2	5
	3	4f	-3, -2, -1, 0, 1, 2, 3	7

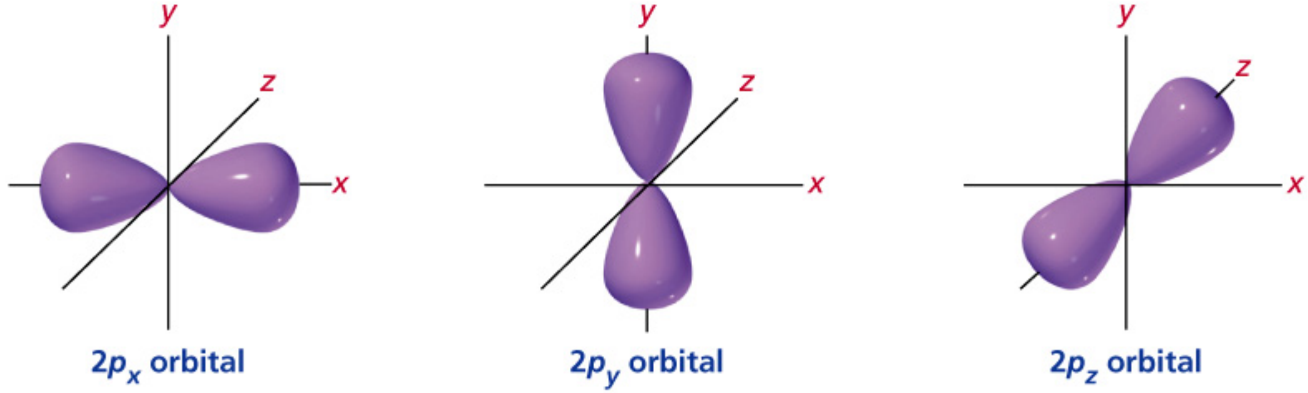
The *s* orbital has a spherical shape centered around the origin of the three axes in space.

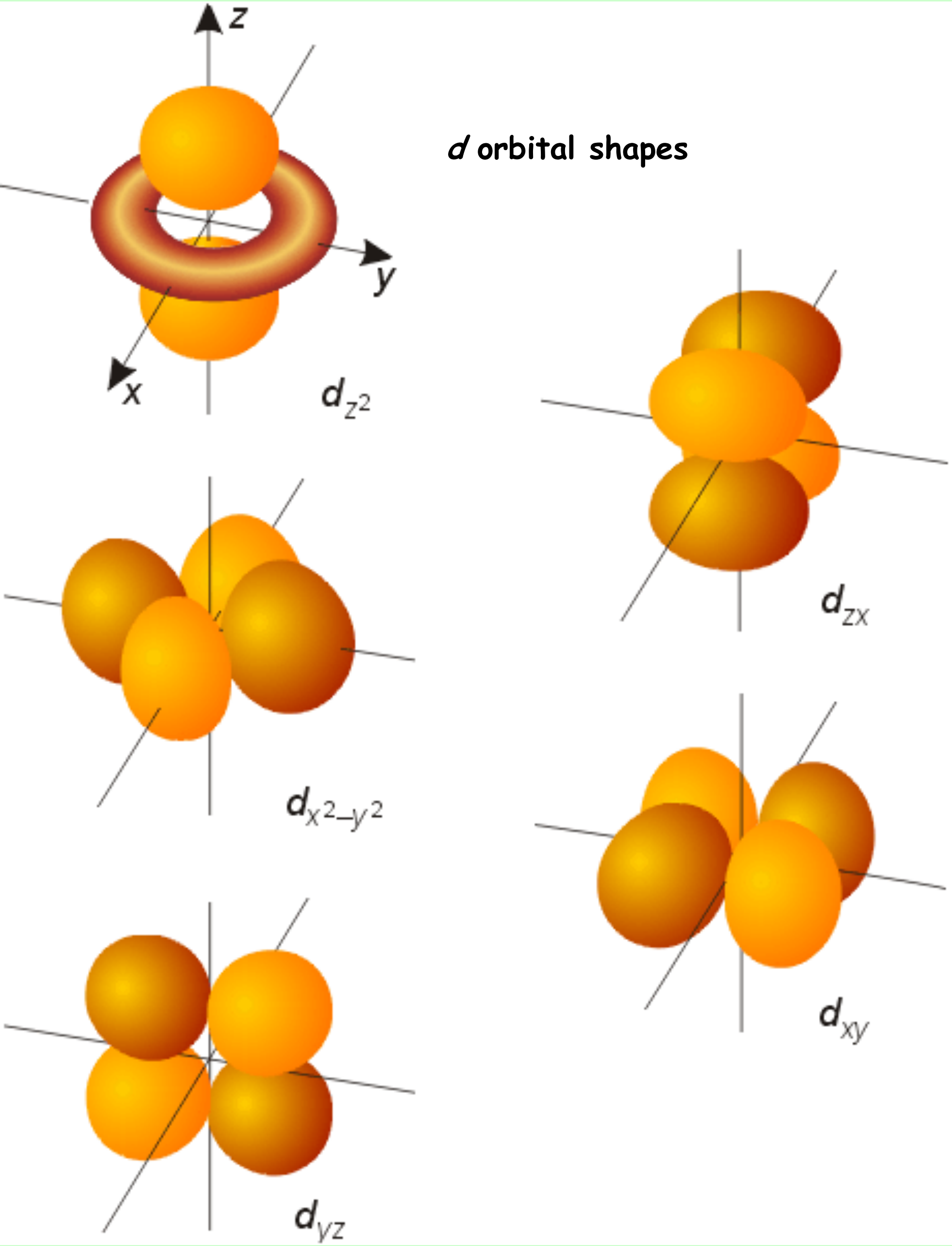


s orbital shape

P orbital shape

There are three dumbbell-shaped *p* orbitals in each energy level above n = 1, each assigned to its own axis (x, y and z) in space.



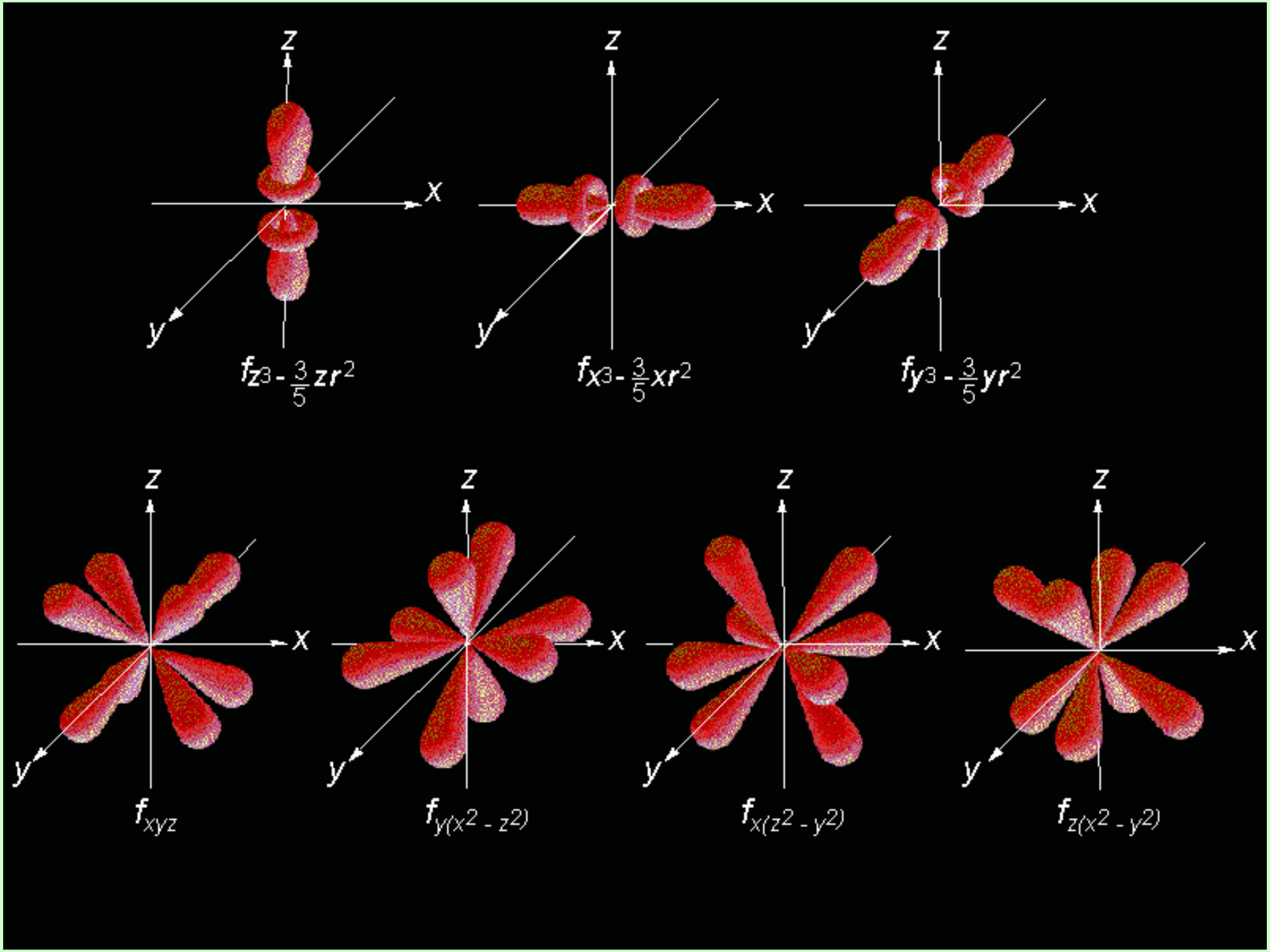


Things get a bit more complicated with the five *d* orbitals that are found in the *d* sublevels beginning with n = 3. To remember the shapes, think of:

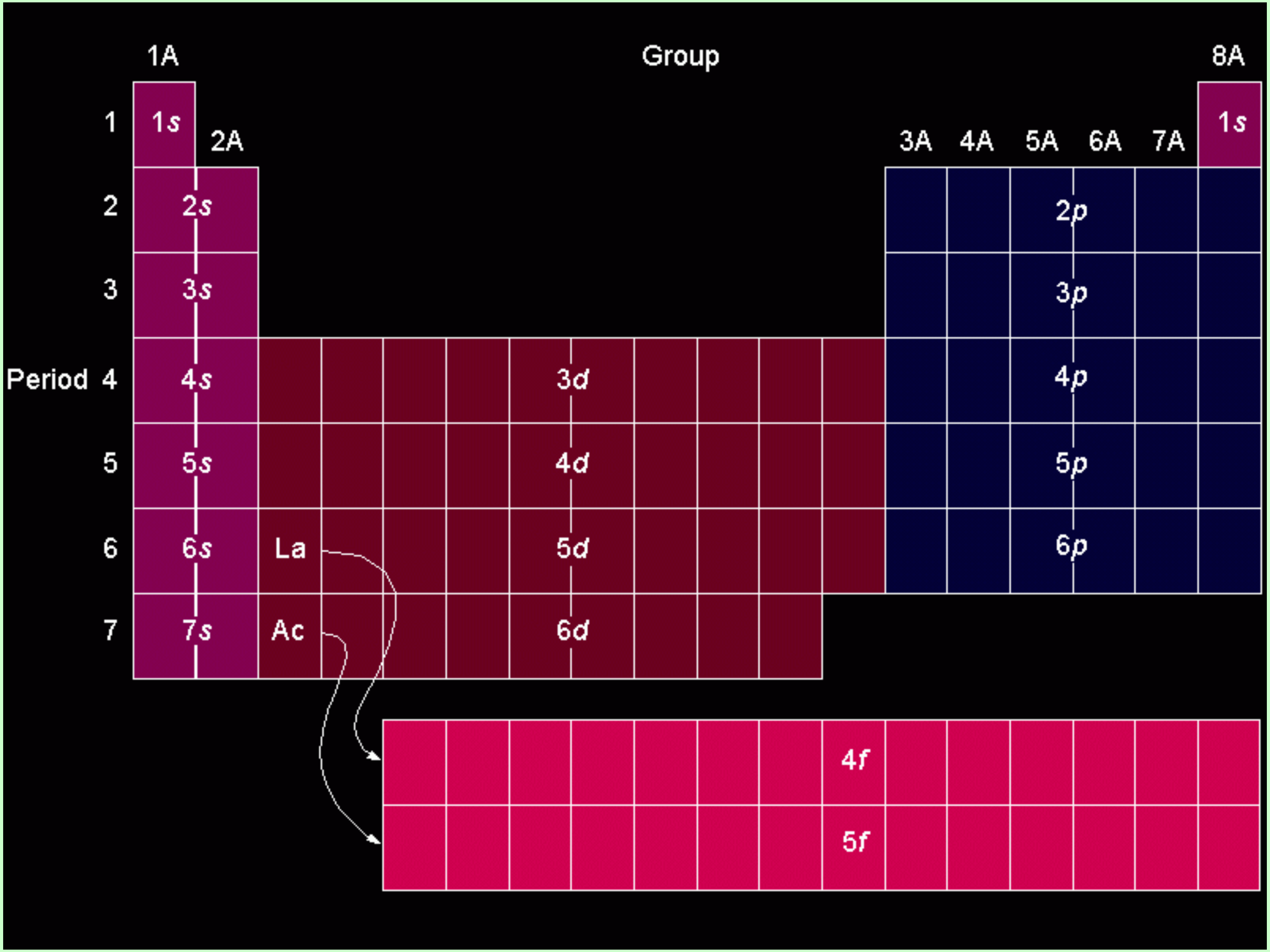
"double dumbells"

…and a "dumbell with a donut"!

Shape of f orbitals



Orbital filling table

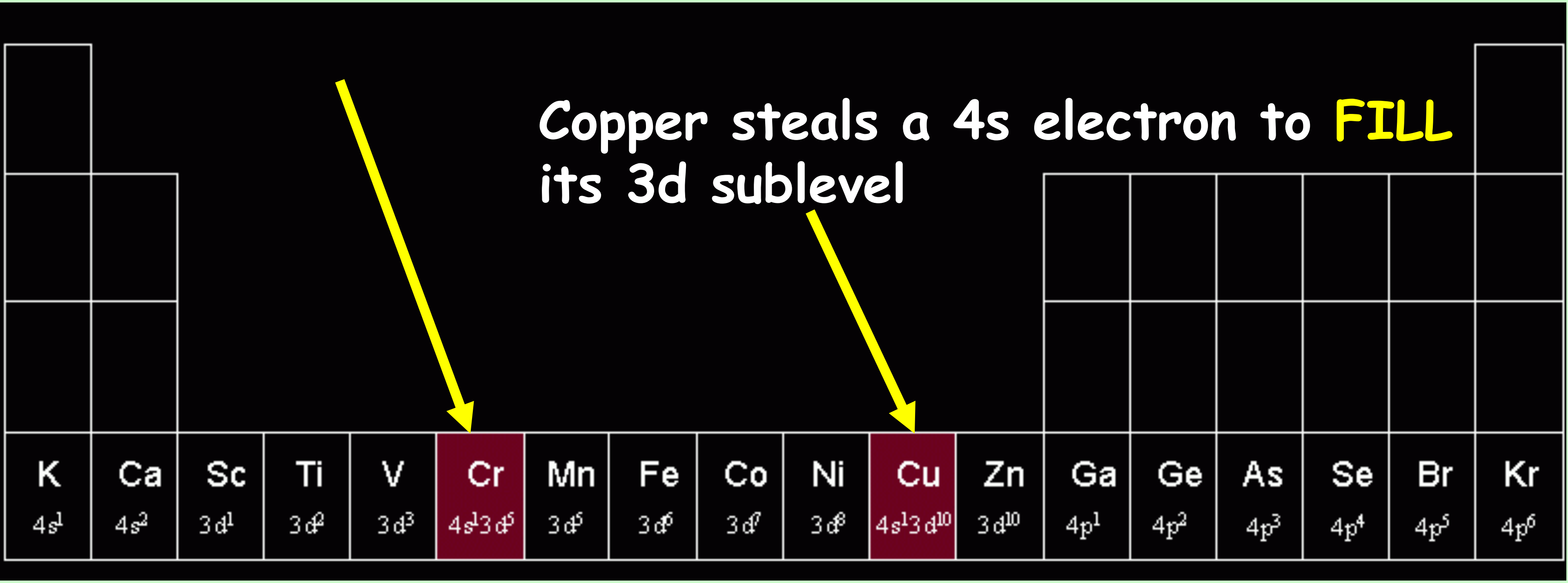


Electron configuration of the elements of the first three series

H $1s^1$							He $1s^2$
Li $2s^1$	Be $2s^2$	B $2p^1$	C $2p^2$	N $2p^3$	O $2p^4$	F $2p^5$	Ne $2p^6$
Na $3s^1$	Mg $3s^2$	Al $3p^1$	Si $3p^2$	P $3p^3$	S $3p^4$	Cl $3p^5$	Ar $3p^6$

Irregular confirmations of Cr and Cu

Chromium steals a 4s electron to half fill its 3d sublevel, no longer part of this class…



Quantum Number Practice

Ex #1: phosphorus

Rule 1: identify the principle energy level, n (same as period)

Rule 2: identify the orbital type, *l* (block the e- is in)

Rule 3: identify the orientation (-*l* to *l*).

Rule 4: 1st half have +1/2 spin, 2nd half have -1/2 spin

P

In period 3

In the p-block

3rd one in ∴ 1

Is 1st half of block, ∴ +1/2

Answer:
(3, 1, 1, +1/2)

Quantum Number Practice

Ex #2: Iron

Rule 1: identify the principle energy level, n (same as period)

Rule 2: identify the orbital type, l (block the e- is in)

Rule 3: identify the orientation ($-l$ to l).

Rule 4: 1st half have +1/2 spin, 2nd half have -1/2 spin

Fe

In period 3

In the d-block

6th one in ∴ -2

Is 2nd half of block, ∴ -1/2

Answer:
(3, 2, -2, -1/2)

Quantum Number Practice

Ex #3: Barium

Rule 1: identify the principle energy level, n (same as period)

Rule 2: identify the orbital type, l (block the e- is in)

Rule 3: identify the orientation ($-l$ to l).

Rule 4: 1st half have +1/2 spin, 2nd half have -1/2 spin

Ba

In period 6

In the s-block

2nd one in ∴ 0

Is 2nd half of block, ∴ -1/2

Answer:
(6, 0, 0, -1/2)

Quantum Number Practice

Ex #4: Tin

Rule 1: identify the principle energy level, n (same as period)

Rule 2: identify the orbital type, / (block the e- is in)

Rule 3: identify the orientation (-/ to /).

Rule 4: 1st half have +1/2 spin, 2nd half have -1/2 spin

Sn

In period 5

In the p-block

2nd one in $\therefore$ 0

Is 1st half of block, $\therefore$ +1/2

Answer:
(5, 1, 0, +1/2)

Quantum Number Practice

Ex #5: Silver

Rule 1: identify the principle energy level, n (same as period)

Rule 2: identify the orbital type, ℓ (block the e- is in)

Rule 3: identify the orientation ($-\ell$ to ℓ).

Rule 4: 1^{st} half have +1/2 spin, 2^{nd} half have -1/2 spin

Ag

In period 4

In the d-block

9^{th} one in $\therefore$ 1

Is 2^{nd} half of block, $\therefore$ -1/2

Answer:
(4, 2, 1, -1/2)

Quantum Number Practice

Ex #6: Oxygen

Rule 1: identify the principle energy level, n (same as period)

Rule 2: identify the orbital type, / (block the e- is in)

Rule 3: identify the orientation (-/ to /).

Rule 4: 1^{st} half have +1/2 spin, 2^{nd} half have -1/2 spin

O

In period 2

In the p-block

4^{th} one in ∴ -1

Is 2^{nd} half of block, ∴ -1/2

Answer:
(2, 1, -1, -1/2)

Electron Energy in Hydrogen
The Bohr Model

$$E_{electron} = -2.178 x 10^{-18} J\left(\frac{Z^2}{n^2}\right)$$

Z = nuclear charge (atomic number)

n = energy level

***Equation works only for atoms or ions with 1 electron (H, He^{+}, Li^{2+}, etc).

Calculating Energy Change, ΔE, for Electron Transitions

$$\Delta E = -2.178 x 10^{-18} J\left(\frac{Z^2}{n_{final}^2} - \frac{Z^2}{n_{initial}^2}\right)$$

Energy must be absorbed from a photon (+ΔE) to move an electron away from the nucleus

Energy (a photon) must be given off (-ΔE) when an electron moves toward the nucleus