The Quantum Mechanical Model of the Atom

SUBLEVELS

The emission spectra of multi-electron atoms suggested that a more complex structure was needed for the ATOM.

EMISSION SPECTRA:

LARGE spaces = NRG differences BETWEEN energy levels

SMALLER spaces = NRG differences WITHIN an energy level

If electrons are changing energy within levels, this suggests that there are sublevels within each level, each with its own slightly different energy.

1924 - Louis de Broglie

- proposed that ***matter has wave-like properties*** - followed from Planck and Einstein's idea that electromagnetic radiation has matter-like properties.
- developed an equation to calculate the wavelength of the matter wave associated with any object, from a bowling ball to an electron.
- de Broglie's theory was proven by experiment -- streams of electrons produced diffraction patterns similar to those produced by electromagnetic radiation, already known to travel in waves.

ORBITALS

1926 - Erwin Schrodinger

- quantum mechanical model of the atom
- described behaviour of electrons in terms of wave functions
- supported by **Werner Heisenberg, in 1927**

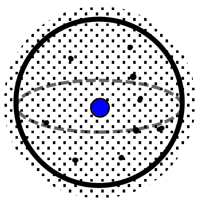
-- demonstrated that it is impossible to know both an electron's position and its momentum at the same time

--*"Heisenberg's uncertainty principle"*

-- cannot talk in terms of certainties, but only in terms of ***probabilities***

-- Schrodinger used a mathematical wave equation to define the probability of finding an electron within an atom

-- multiple solutions to this wave equation -- ***solutions were known as wave functions, or orbitals.***



1s sublevel - probability of finding an electron near the nucleus is high, but extremely small when it is far away from nucleus, but never quite reaches zero.

The bold circle encompasses 95% of the probability the electron will be found in the spherical shape.

SHAPES of orbitals are cloud-like

- shape of each cloud is based on probability -- where an electron spends most of its time

ATOMIC STRUCTURE AND THE PERIODIC TABLE

- **QUANTUM MECHANICS** - new understanding of property of matter and link between electron arrangement of atoms and the structure of the periodic table

- **Bohr model of electron ORBITS vs. Modern model of electron ORBITALS** (region of space around nucleus where an electron is likely to be found)

(BOHR'S) ORBITS	(MODERN) ORBITALS
2-D path	3-D region in space
fixed distance from nucleus	variable distance from nucleus
circular or elliptical path	no path; varied shape of region
$2n^2$ electrons per orbit	2 electrons per orbital

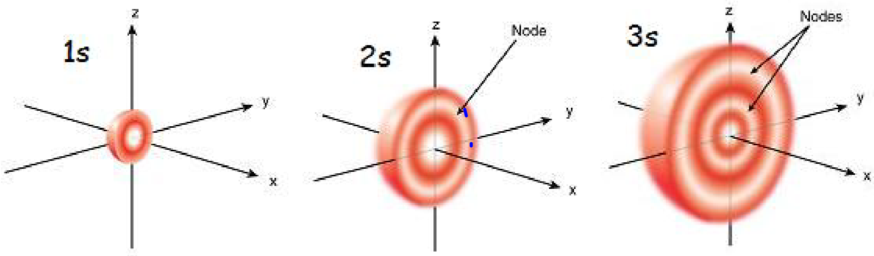
energy level (n)	number of orbitals (n^2)	number of electrons ($2n^2$)	relates to...
1	1	2	**PERIOD 1 elements** H & He
2	4	8	**PERIOD 2 elements** (groups 1A to 8A)
3	9	18	**PERIOD 3 elements** (groups 1A to 8A; 1st row transition elements)
4	16	32	**PERIOD 4 elements** (groups 1A to 8A; 1st row inner transition elements; 2nd row transition elements)
...	...	...	

SHAPES OF ORBITALS

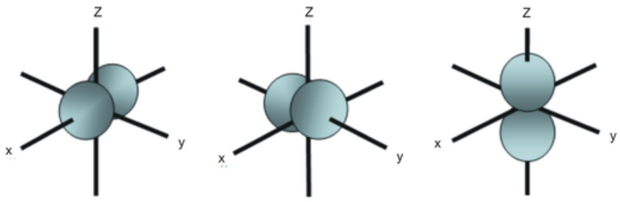
Overall shape of an atom is the combination of all its orbitals

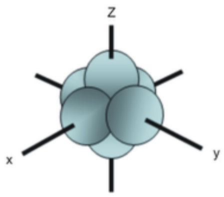
- tends to be spherical, but not spherical in the sense of the "s" orbital
- shapes are solutions to mathematical equations -- describing the motion and position of electrons in terms of probabilities.
- think of the shapes as "containers" which electrons "occupy"

1 s - orbital



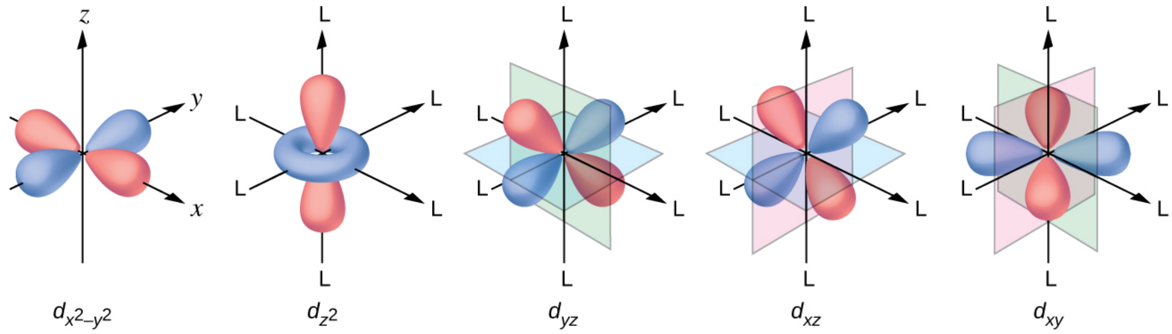
3 different p - orbitals

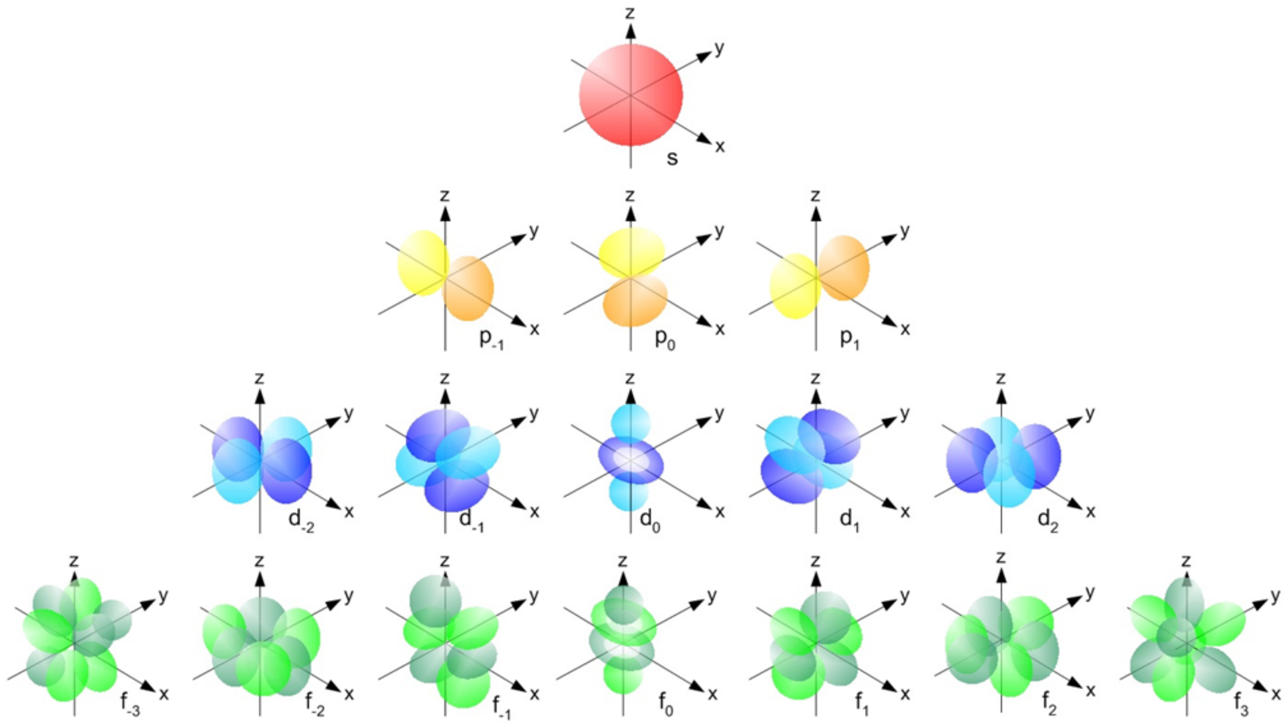




when all 3 orbitals are combined

5 different d - orbitals




s
p_{-1}
p_0
p_1
d_{-2}
d_{-1}
d_0
d_1
d_2
f_{-3}
f_{-2}
f_{-1}
f_0
f_1
f_2
f_3

PART 1: QUANTUM NUMBERS for ELECTRONS in ATOMS

1. Principle Quantum Number (n)

> **ENERGY LEVEL** of atomic orbital

> 1, 2, 3, 4, ...

> corresponds with **rows** in periodic table

2. Second Quantum Number (l)

> **SHAPE** of an atomic orbital

> from 0 to $n - 1$

> corresponds with **columns** in periodic table

$l = 0$	*denoted by s*
$l = 1$	*denoted by p*
$l = 2$	*denoted by d*
$l = 3$	*denoted by f*

3. Third Quantum Number (m_l)

> **ORIENTATION** of an atomic orbital

> from $-l$ to l.

> If $l = 2$, then m_l = -2, -1, 0, 1, 2.

4. Fourth Quantum Number (m_s)

> **SPIN** of an electron

> each orbital can hold only 2 electrons

> opposite spins

> +1/2 or -1/2

n	l	orbital designation	m_l	# of orbitals	# 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

① QUANTUM NUMBERS

1. State the quantum numbers for each description.

   A) platinum

   B) chlorine

   C) krypton

   D) polonium, astatine, radon

   E) gallium, selenium

   F) alkaline earth metals

   G) beryllium, oxygen, fluorine, neon

   H) copper, silver, gold

2. Use the given quantum information to identify the element(s).

   A) $n = 3,\ l = 1,\ m_l = 1,\ m_s = +\frac{1}{2}$

   B) $n = 4,\ l = 2,\ m_l = -1,\ m_s = -\frac{1}{2}$

   C) $n = 2,\ l = 1,\ m_l = -1$

   D) $n = 5,\ l = 3,\ m_l = 1,\ m_s = +\frac{1}{2}$

   E) $n = 2,\ l = 0,\ m_s = -\frac{1}{2}$

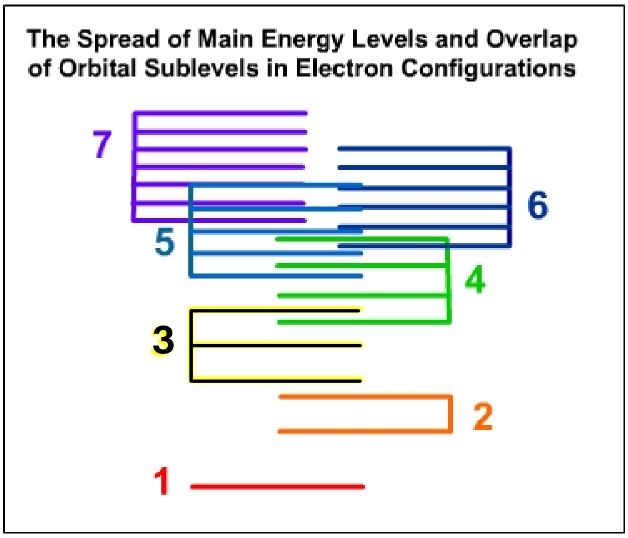
   F) $n = 4,\ l = 3,\ m_l = 3$

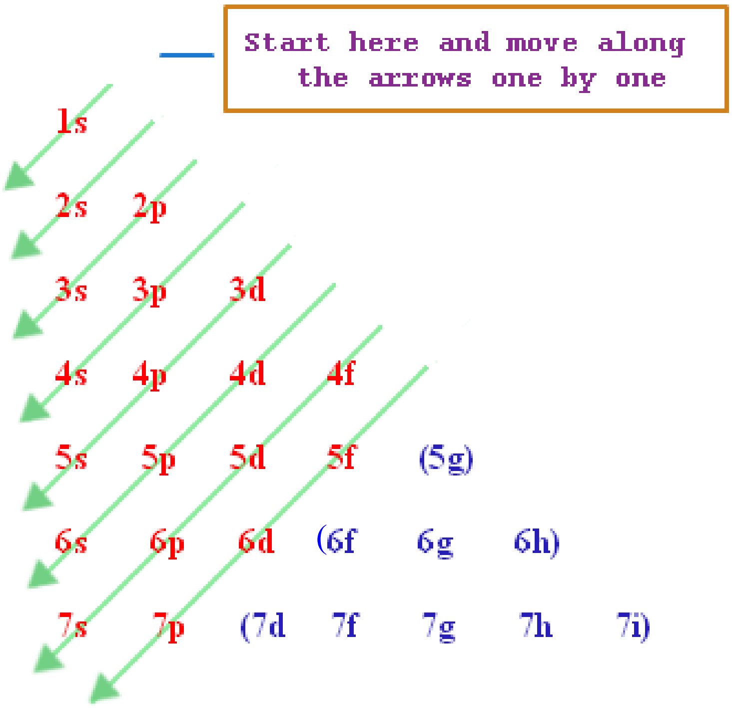
   G) $n = 4,\ l = 2,\ m_s = \frac{1}{2}$

   H) $n = 5,\ m_l = -1$

PART 2: WRITING ELECTRON CONFIGURATIONS

-- energy levels are listed in order of increasing energy





RULES FOR FILLING ENERGY LEVELS WITH ELECTRONS:

1. No two electrons in an atom can have the same 4 quantum numbers.

- ***Pauli Exclusion Principle***
- "Everyone is unique."

2. Fill lowest energy level first and then work upwards until the limit on the number of electrons for the particle is reached.

- ***Aufbau Principle***
- "When you get on the bus, find the first vacant seat."

3. Place one electron per orbital at a given energy level before doubling up electrons.

- ***Hund's Rule***
- "*Dinnertime rule - each person at the table gets one serving before anyone gets a second serving."*

4. Anions = add on electrons

Cations= subtract electrons from orbital with highest "n" value

5. Maximum number of electrons per orbital: s = 2, p = 6, d = 10, f = 14

NOTE: All electrons in an atom are in the lowest possible energy levels -- in this ***ground state***, the atom is most stable.

② ELECTRON CONFIGURATION

nl^x ... n = energy level (period)

l = orbital shape

x = number of electrons in the orbital

- the distribution of electrons of an atom or molecule in atomic or molecular orbitals. For example, the electron configuration of the neon atom is $1s^2\ 2s^2\ 2p^6$, using the notation explained above.

1. For each atom/ion,
   - Write the complete electron configuration
   - Write the condensed electron configuration

A) calcium

B) sulfur

C) chlorine

D) oxide ion

E) manganese

F) cuprous ion

G) iodine

H) rubidium ion

I) gadolinium

J) auric ion

K) $n = 5,\ l = 2,\ m_l = -1,\ m_s = -\frac{1}{2}$

2. Identify the element.

A) [Ne] $3s^2 3p^4$

B) [He] $2s^2 2p^1$

C) [Ar] $3d^{10} 4s^2 4p^2$

D) [Ne] $3s^2 3p^3$

E) [Kr] $4d^5 5s^2$

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

G) [Xe] $4f^{14} 5d^{10} 6s^2 6p^5$

H) [Rn] $5f^{10} 7s^2$

I) [Ar] $3d^8 4s^2$

J) [Xe] $4f^{14} 5d^4 6s^2$

K) [Kr] $4d^1 5s^1$ -- determine the wavelength of energy absorbed by the excited electron, using Rydberg's formula for a hydrogen atom.

PART 3: ORBITAL DIAGRAMS

- Orbital diagrams are pictorial representations of the electrons in an atom.

- An orbital diagram uses boxes with arrows to represent the electrons in an atom. Each box in an orbital diagram represents an orbital. Arrows are drawn inside the boxes to represent electrons. Two electrons in the same orbital must have opposite spin so the arrows are drawn pointing in opposite directions.

Three rules are useful in forming orbital diagrams:

1. *AufBau Principle*, each electron occupies the lowest energy orbital.

2. *Pauli Exclusion Principle* says that only two electrons can fit into a single orbital and they must have opposite spin.

3. *Hund's rule* states that every orbital in a subshell is singly occupied with one electron before any one orbital is doubly occupied, and all electrons in singly occupied orbitals have the same spin.

$\square$ = 1 orbital

Therefore, s orbitals contains 1 box.
p orbitals contains 3 boxes.
d orbitals contains 5 boxes.
f orbitals contains 7 boxes.

1. Draw the orbital diagram for each atom. [Consider only the valence shell of the atom.]

A) hydrogen atom

B) helium atom

C) nitrogen atom

D) bromine atom

E) silicon atom

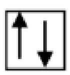
F) iron atom and the ferrous ion

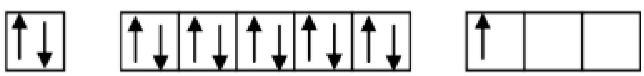
EXCEPTIONS: copper and chromium

COPPER: Expected:

Actual:

2. Name all elements with the given configuration.

A) 

B) 

BRINGING IT ALL TOGETHER!

1. Identify the element, then illustrate the element using the other representations.

A) $n = 5,\ l = 2,\ m_l = -1,\ m_s = +\frac{1}{2}$

B) [Kr] $4d^2 5s^2$

C)