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Atomic Models and Properties of Atoms

Historically, scientists have used their knowledge of atomic properties to develop and refine atomic models. Today, this knowledge is applied to various research techniques.

Scientists can now determine colour patterns of ancient bird feathers by identifying elements present in fossils of the birds.

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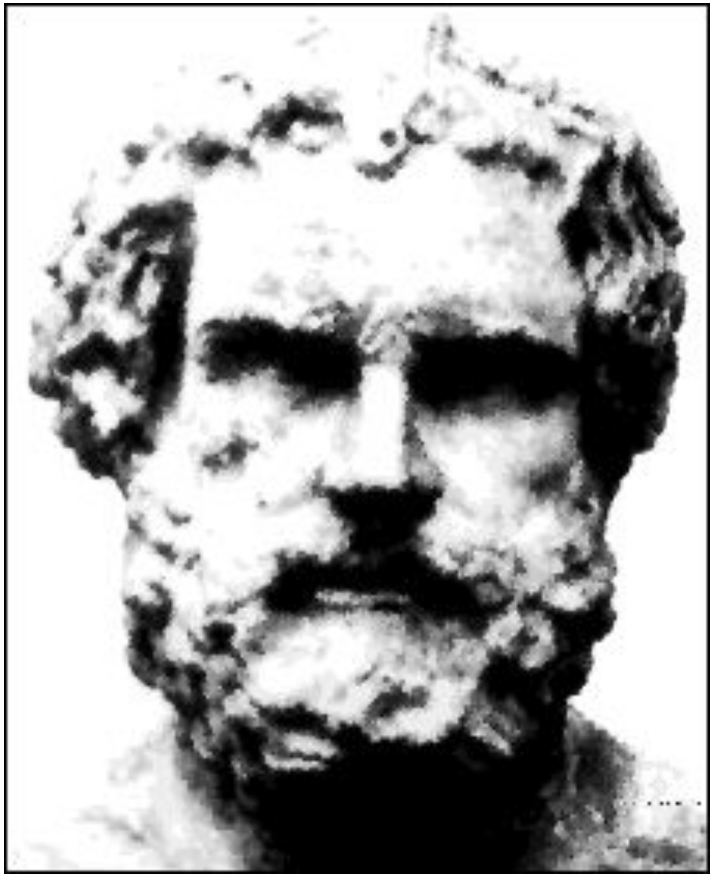
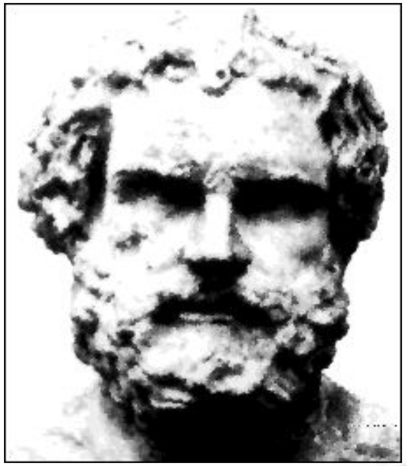
Democritus

This is the Greek philosopher Democritus who began the search for a description of matter more than 2400 years ago.

He asked: Could matter be divided into smaller and smaller pieces forever, or was there a limit to the number of times a piece of matter could be divided?



Atomos

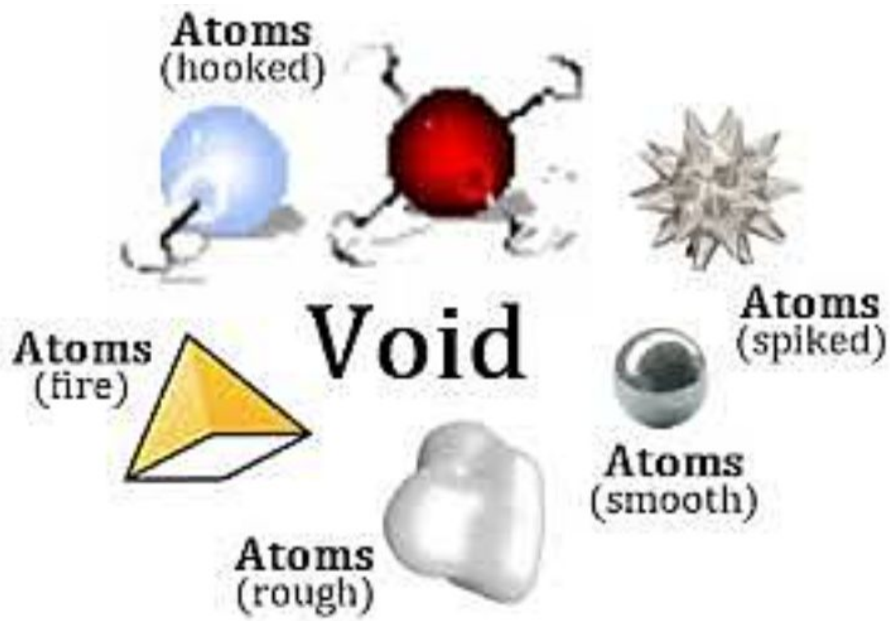


His theory: Matter could not be divided into smaller and smaller pieces forever, eventually the smallest possible piece would be obtained.

This piece would be indivisible.

He named the smallest piece of matter “atomos,” meaning “not to be cut.”

Atomos



- To Democritus, atoms were <u>small</u>, hard particles that were all made of the same material but were <u>different</u> shapes and sizes.
- Atoms were <u>infinite</u> in number, always moving and capable of joining together.

This theory was ignored and forgotten for more than *2000* years!

START HERE P3 -> Do nature of sci activity

3.1 Developing a Nuclear Model of the Atom

We will take a look at each of these models on the coming slides

Dalton's model (1808)

↓

Thomson's model (1904)

↓

Rutherford's model (1911)

↓

Bohr's model (1913)

↓

quantum mechanical model (present)

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Reviewing the Atomic Models of Dalton and Thomson

John Dalton's model of the atom: The Indivisible Atom

- marked the beginning of a new way of explaining matter
- matter was described as being composed of small, indivisible spheres, which Dalton called atoms

Dalton envisioned atoms as hard, solid spheres.

Why did the discovery of subatomic particles like electrons require a new atomic model?

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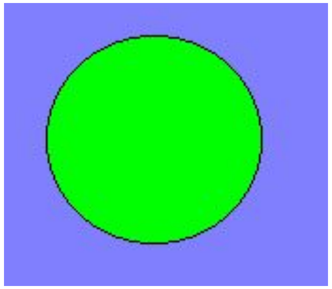
Subatomic particles showed the atom WAS divisible and made of smaller particles.

Dalton's Model

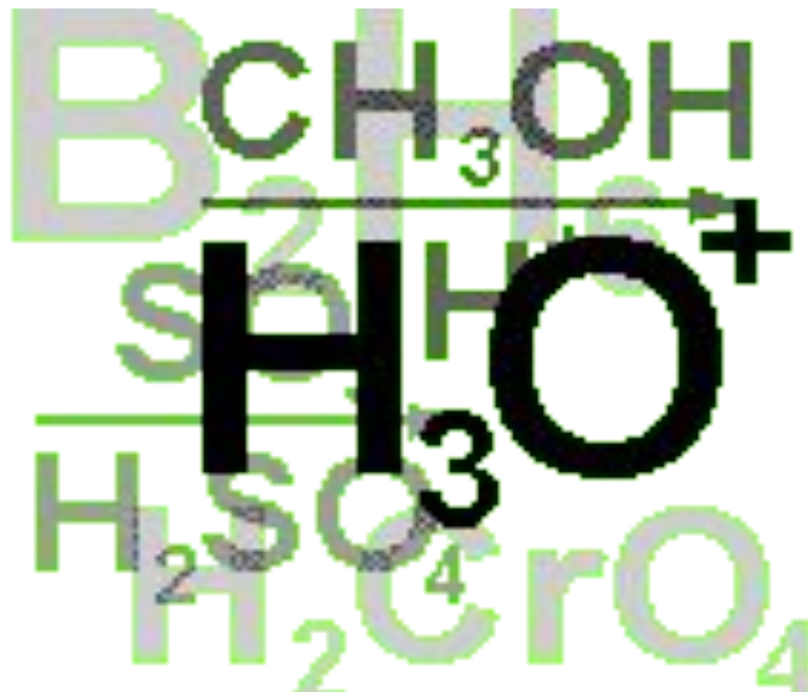
In the early 1800s, the English Chemist John Dalton performed a number of experiments that eventually led to the acceptance of the idea of atoms.

Dalton's Theory

1. All matter is made of tiny indivisible and indestructible particles called atoms.
2. Atoms of the same element are exactly alike (properties, mass, etc).
3. Atoms of different elements are different in properties and mass.
4. Atoms of different elements (and a few with themselves), combine in small whole number ratios to form compounds
5. In chemical reactions, atoms are not created or destroyed. They are rearranged or combined.



This theory became one of the foundations of modern chemistry.



Thomson's Plum Pudding Model

In <u>1897</u>, the English scientist J.J. Thomson provided the first hint that an atom is made of even <u>smaller</u> particles.

Thomson Model

Thomson studied the passage of an electric current through a gas.

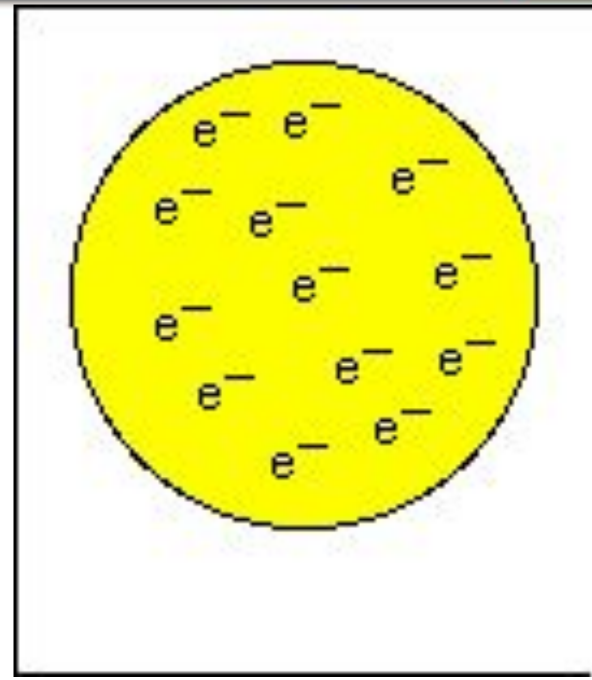
As the current passed through the gas, it gave off rays of negatively charged particles (ie….).

Start here P2

Thomson Model

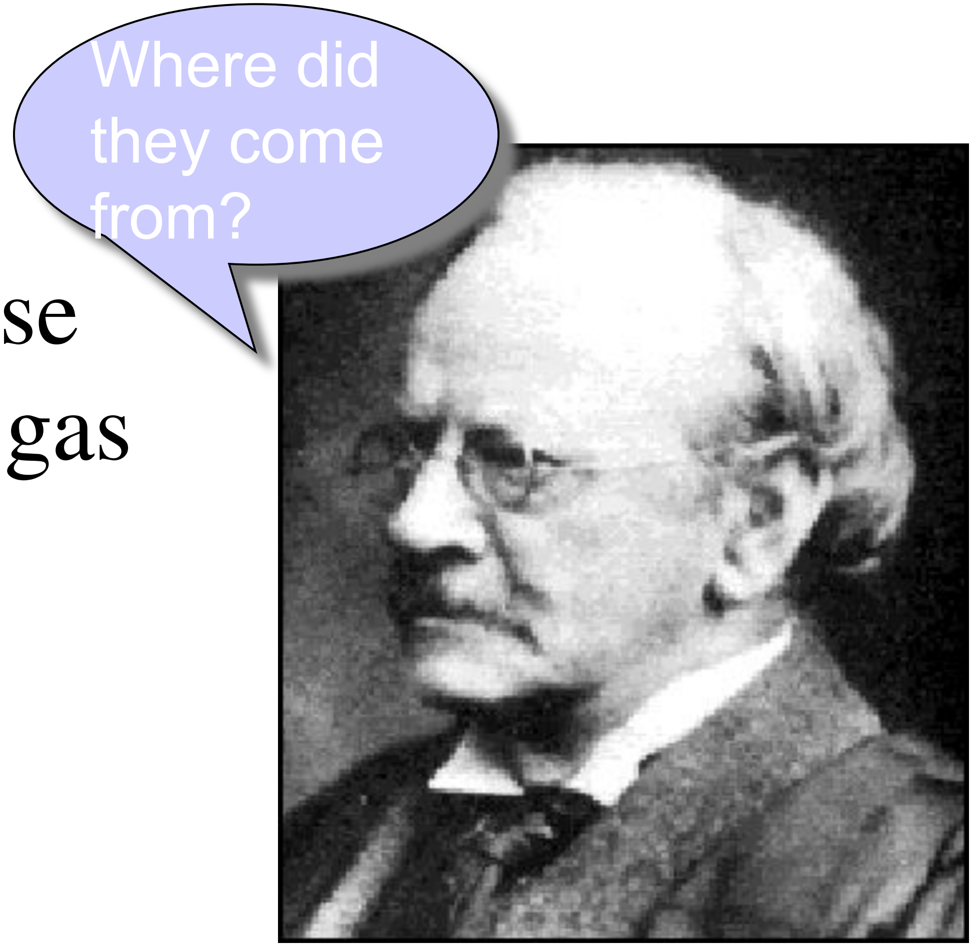
"Plum Pudding"

1. The atom is a spherical cloud of positive charge with negatively charged electrons embedded in it
2. The amount of positive charge equals the amount of negative charge, so the entire atom is neutral.



Thomson Model

This surprised Thomson, because the atoms of the gas were uncharged. Where had the negative charges come from?



Thomson concluded that the negative charges came from *<u>within</u>* the atom.

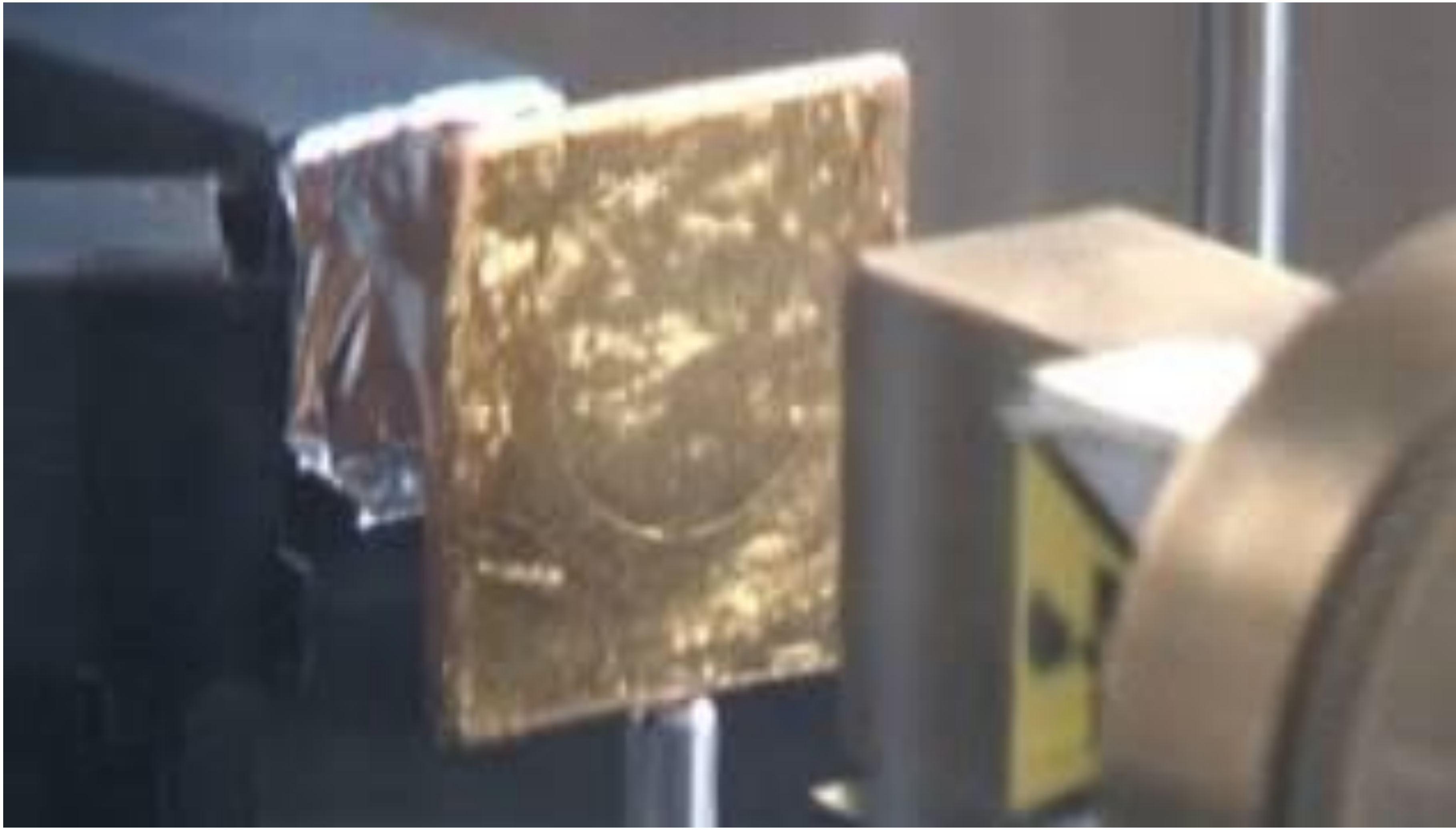
A particle smaller than an atom <u>had to exist</u>.

The atom was <u>divisible!</u>

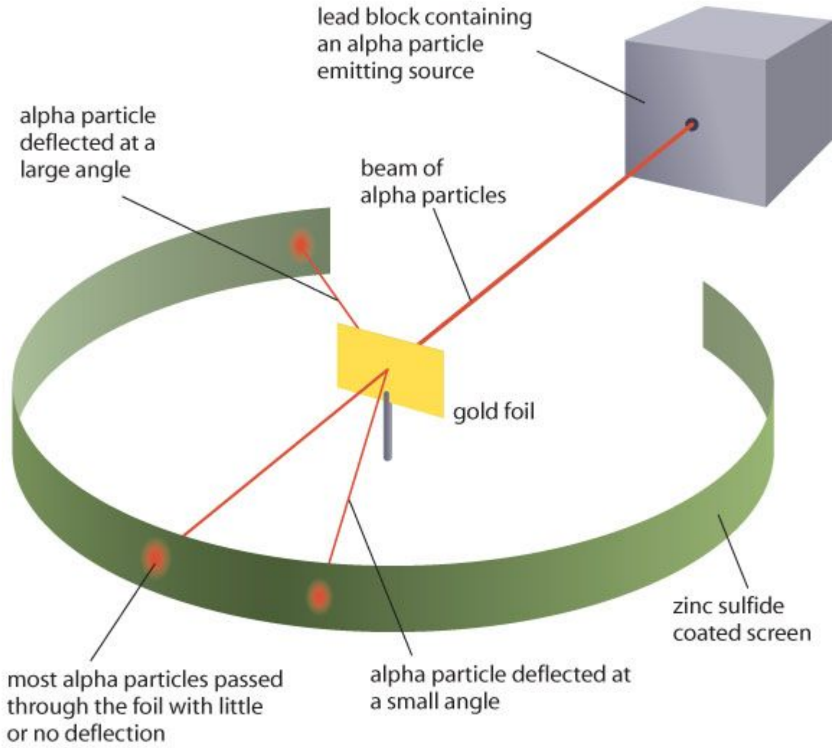
Thomson called the negatively charged “<u>corpuscles,</u>” today known as <u>electrons</u>.

Since the gas was known to be neutral, having no charge, he reasoned that there must be <u>positively</u> charged particles in the atom.

But he could never find them.



Rutherford's Gold Foil Experiments



Alpha (positively charged, 2p+2n) particles were aimed at gold foil. The scattering of the alpha particles was monitored.

Expectation (Thomson's model):
- particles pass through or some slightly deflected

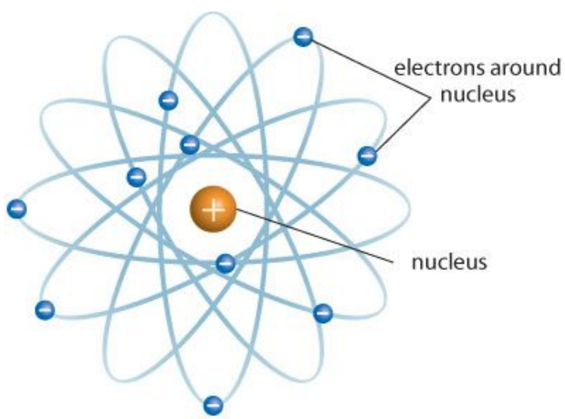
Observation:
- some particles deflected at large angles

Rutherford's experimental observations required a new atomic model.

Rutherford's Nuclear Atomic Model

Rutherford's model of the atom:

- large deflections of particles proposed to be due to presence of an electric field at the centre of the atom (he knew positive repelled positive)
- an atom has a positively charged nucleus at the centre with electrons scattered in motion surrounding the nucleus



The nuclear, or planetary model, of the atom.

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Rutherford's Gold Foil Expt Conclusions

1. The atoms is mostly empty space
2. Most of the mass is concentrated in a small, dense, nucleus
3. Electrons move around the nucleus like planets around the sun

Moseley and the Atomic Number

- Prior to Mosely, the atomic number was thought of as a somewhat arbitrary number related to, but separate from, atomic mass
- Henry Moseley found that certain lines in the X-ray spectrum of each element moved the same amount (linear relationship) each time the atomic number increased by one.
- This yielded, for the first time, a measurable property of the nucleus that was directly related to atomic number
- IMPORTANT TAKEAWAY: The number of protons determines the identity of the element – the atomic number Z

Atomic notation and Isotopes

Z = atomic number   A = atomic mass

What is atomic mass?

How can we calculate the number of neutrons?

If two atoms have the SAME atomic number (Z) but different atomic masses (A), they are….?

How will their properties compare?

What if they have DIFFERENT atomic numbers (Z) but the SAME atomic masses (A)?

ANSWERS: Atomic notation and Isotopes

Z = atomic number A = atomic mass

What is atomic mass? Number of protons + Neutrons

How can we calculate the number of neutrons?

Neutrons = Atomic mass - atomic number

If two atoms have the SAME atomic number (Z) but different atomic masses (A), they are….? Isotopes (SAME element but diff number of neutrons

How will their properties compare? Isotopes have the SAME properties

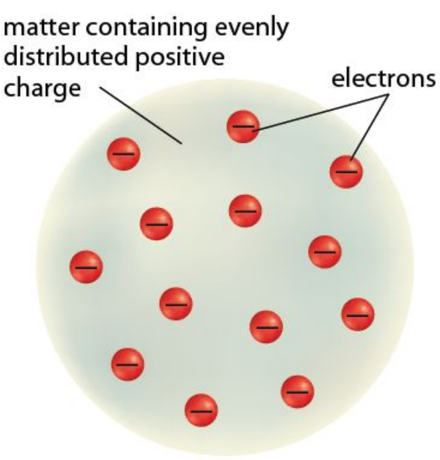
What if they have DIFFERENT atomic numbers (Z) but the SAME atomic masses (A)? They are DIFFERENT elements and the same mass is just a coincidence.

End Here → Next The Bohr_Rutherford Model PP (The Nuclear model)

Reviewing the Atomic Models of Dalton and Thomson

J.J. Thomson's model of the atom:

- incorporated his discovery of the electron, using cathode ray tubes
- an atom is a positively charged spherical mass with negatively charged electrons embedded within



Thomson's "plum pudding" model of the atom.

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NEXT TIME:

Atomic Numbers and Isotopes

Towards the development of the Quantum Model of the Atom

The Limitations of Rutherford's Atomic Model

Based on the understanding of physics at the time, for an electron in motion around a central core:

- radiation must be emitted, so it was expected that a continuous spectrum of light energy was being given off
- because of radiation, the electron would lose energy and its orbit would decrease until it spiraled into the nucleus, destroying the atom

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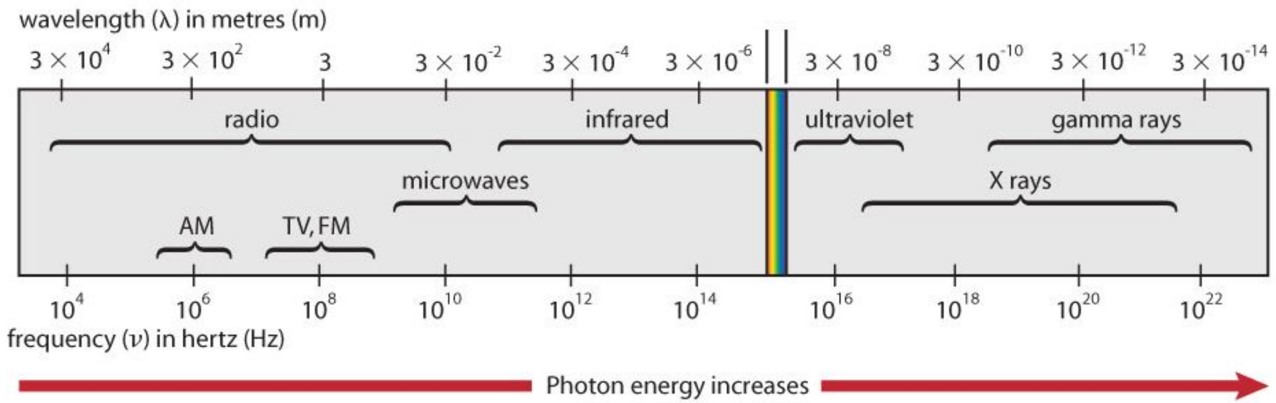
Rethinking Atomic Structure Based on the Nature of Energy

Light is one form of **electromagnetic radiation,** which travels through space as waves

Electromagnetic waves:

- have ***frequency***, *wavelength*, and *amplitude*
- interact with matter in discrete particles called **photons**



Electromagnetic Spectrum

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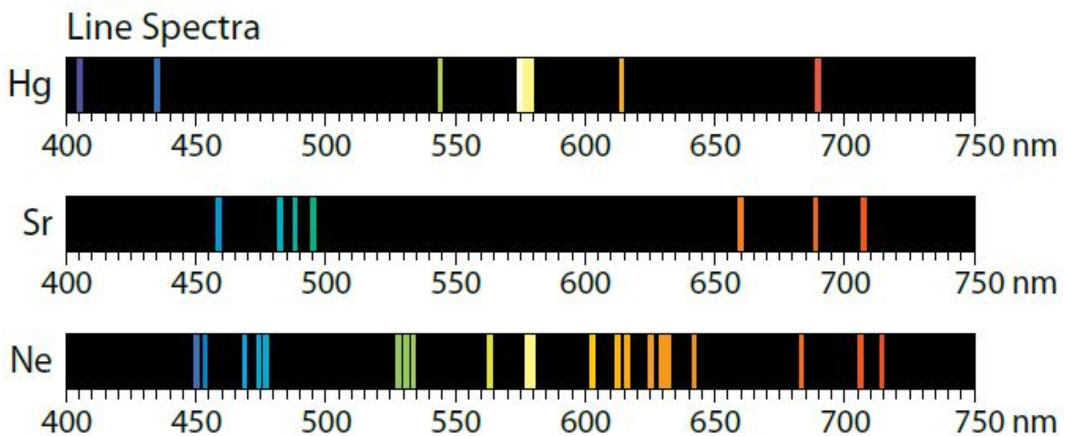
Atomic Spectra

When atoms are excited due to absorption of energy, they emit light as they lose energy and return to a non-excited state.

Atoms of each element emit light of particular wavelengths called a **line spectrum** or **emission spectrum**.



Each element has a characteristic line spectrum.

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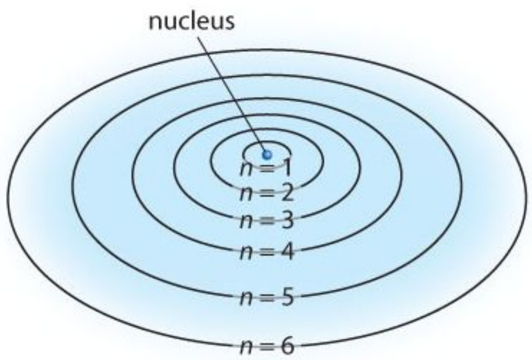
The Bohr Model of the Hydrogen Atom

Niels Bohr set out to explain the stability of the **nuclear model** of the atom. In this model, electrons

- are in circular orbits
- can only exist in certain "allowed" orbits or energy levels (energy of electrons is *quantized*)
- do not radiate energy while in one orbit
- can jump between orbits by gaining or losing a specific amount of energy



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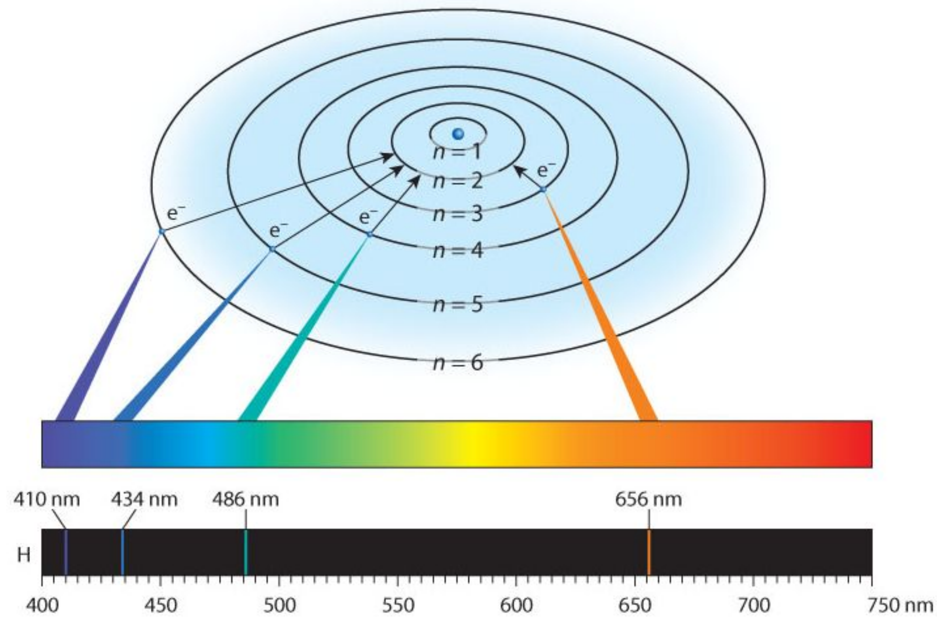
Bohr's Atomic Model Explains the Line Spectrum of Hydrogen

- Calculated wavelengths of the possible energies of photons that could be emitted from an excited hydrogen atom (transitions from *n* = 6, 5, 4, and 3 to *n* = 2) corresponded with hydrogen's visible line spectrum

Limitations

- could only explain single-electron systems (H, He^{+}, Li^{2+})



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Section 3.1 Review

Section 3.1 The Nuclear Model of the Atom

Building on and extending from the work of scientists who came before them as well as their peers, Ernest Rutherford and Niels Bohr developed atomic models that, today, are referred to as nuclear and planetary models of the atom.

Key Terms

electromagnetic radiation	nuclear model
emission spectrum or line spectrum	photon
frequency	quantum

Key Concepts

- Historically, the development of and modifications to the atomic model have been the result of experimental evidence and new ideas about the nature of matter and energy.
- Thomson's discovery of the electron disproved Dalton's model of the atom as a solid, indivisible sphere. Instead, Thomson proposed that the atom existed as a positively charged sphere, with enough negatively charged electrons embedded in it to balance the overall charge on the atom.
- Observations and inferences made by Rutherford led to a nuclear model of the hydrogen atom. This model is still the most commonly depicted, with negatively charged electrons orbiting around a central positively charged nucleus.
- Bohr's model of the atom refined the Rutherford model, incorporating the concept that, like light, electrons in atoms could have only certain amounts of energy and, therefore, could exist in only specific orbits around the nucleus. Each allowed orbit had a specific amount of energy and a specific radius.

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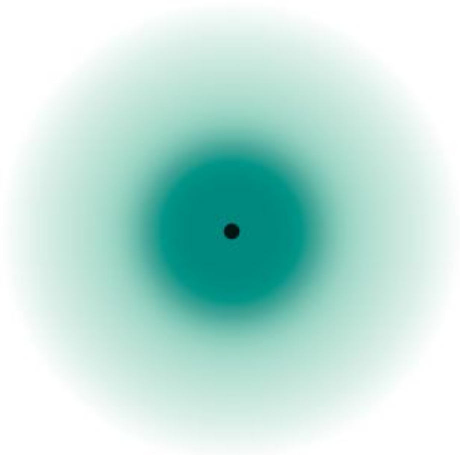
3.2 The Quantum Mechanical Model of the Atom

Today's **quantum mechanical model of the atom** incorporates the wave properties of electrons.

Wave functions, initially described by Erwin Schrodinger, represent a region in space around a nucleus where an electron will be found. This region of space is called an **atomic orbital**



An electron density diagram represents an atomic orbital.

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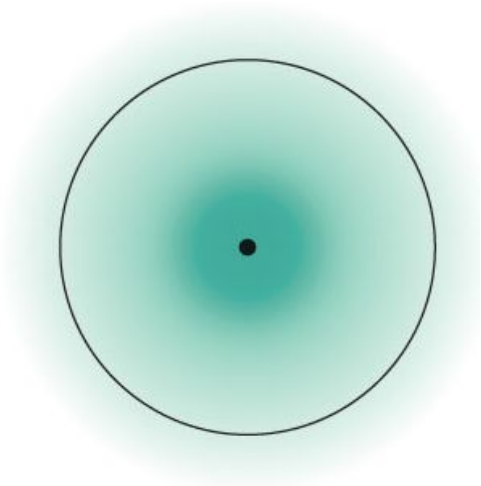
The Quantum Mechanical Model of the Atom

Atomic orbitals can be visualized as "fuzzy clouds"

- The higher the density of the "cloud," the higher the probability of finding an electron at that point.
- The cloud has no definite boundary.
- The region where an electron will spend 90 percent of its time is depicted by drawing a circle.



The circle does not represent a real boundary.

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Quantum Numbers Describe Orbitals

Electrons in the quantum mechanical model of the atom are described using **quantum numbers**.

Three quantum numbers describe the distribution of electrons in the atom and a fourth describes the behaviour of each electron.

Symbols for the four quantum numbers:

n l m_l m_s

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The Principle Quantum Number, *n*

- Is the first quantum number
- Describes the energy level, or **shell**, of an orbital
- All orbitals with the same *n* value are in the same shell
- The larger the *n* value, the larger the size of the shell
- Values can range from $n = 1$ to $n = \infty$

$n = 1$	first shell
$n = 2$	second shell
$n = 3$	third shell
$n = 4$	fourth shell

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The Orbital-Shape Quantum Number, l

- Is the second quantum number
- Describes the shape of an orbital
- Refers to energy **sublevels**, or subshells
- Values depend on the value of n. They are positive integers from 0 to $(n – 1)$
- Each value is identified by a letter

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

An energy sublevel is identified by combining n with the orbital letter. For example, $n = 2$, $l = 1$: 2p sublevel

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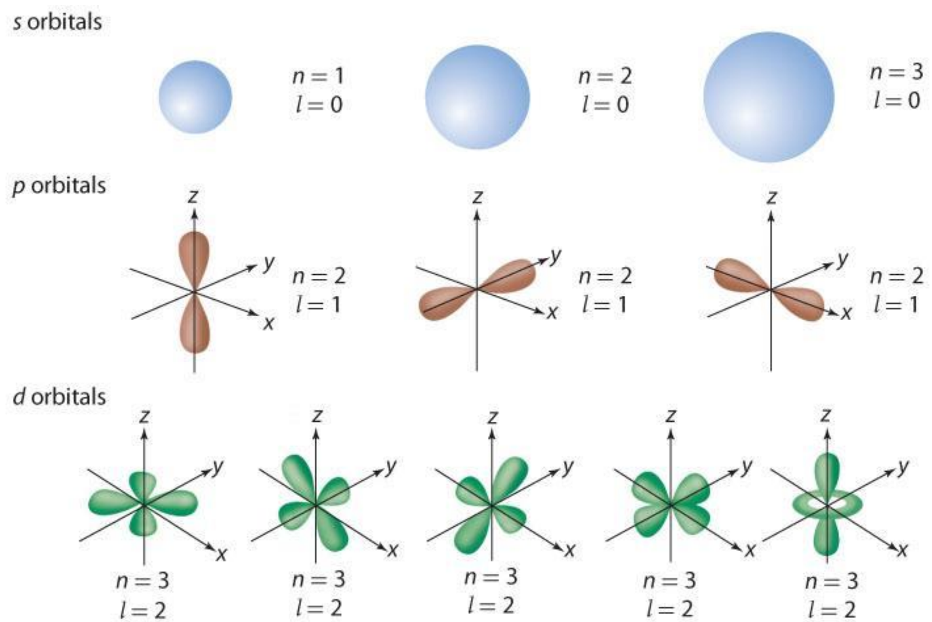
The Magnetic Quantum Number, m_l

- Is the third quantum number
- Indicates the orientation of the orbital in space
- For a given l there are $(2l+1)$ values for m_l
- The total number of orbitals for an energy level is n^2



s, *p*, and *d* orbitals have characteristic shapes.

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The Spin Quantum Number, m_s

- Is the fourth quantum number
- Specifies the orientation of the axis of electron spin
- Two possible values: +½ or –½

To summarize:

Name	Symbol	Allowed Values	Property
Principal (shell)	n	Positive integers (1, 2, 3, etc.)	Orbital size and energy level
Orbital-shape (subshell)	l	Integers from 0 to $(n - 1)$	Orbital shape (l values 0, 1, 2, and 3 correspond to *s*, *p*, *d*, and *f* orbitals)
Magnetic	m_l	Integers from $-l$, to $+l$	Orbital orientation
Spin	m_s	$+\frac{1}{2}$ or $-\frac{1}{2}$	Spin orientation

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Identifying Electrons Using Sets of Quantum Numbers

According to the **Pauli exclusion principle**:

- an orbital can have a maximum of two electrons
- two electrons in an orbital must have opposite spins

No two electrons of an atom have the same set of four quantum numbers.

Atom	Electron	Quantum Numbers
hydrogen	Lone	$n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$
helium	First	$n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$
	Second	$n = 1, l = 0, m_l = 0, m_s = -\frac{1}{2}$

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LEARNING CHECK

What is the set of quantum numbers for an electron in a 2*s* orbital?

Answer on the next slide

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LEARNING CHECK

$n = 2, l = 0, m_l = 0, m_s = +½$

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Section 3.2 Review

Section 3.2 The Quantum Mechanical Model of the Atom

New ideas and experimental evidence about the wave nature of particles led to a new, revolutionary atomic model—the quantum mechanical model of the atom.

Key Terms

atomic orbital

magnetic quantum number, m_l

orbital-shape quantum number, l

principal quantum number, n

Pauli exclusion principle

quantum mechanical model of the atom

quantum numbers

shell

spin quantum number, m_s

sublevel

Key Concepts

- According to the quantum mechanical model of the atom, electrons have both matter-like and wave-like properties.
- The position and momentum of atoms cannot both be determined with certainty, so the position is described in terms of probabilities.
- An orbital represents a mathematical description of the region of space in which an electron has a high probability of being found.
- The first three quantum numbers describe the size, energy, shape, and orientation of an orbital. The fourth quantum number describes the orientation of the axis around which the electron is spinning.

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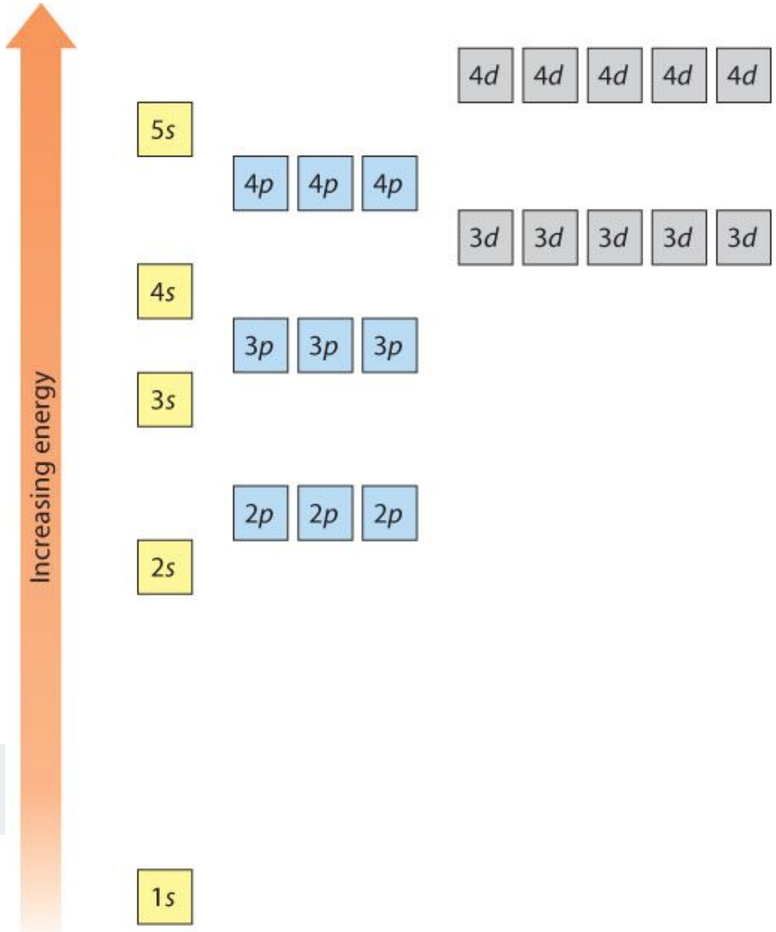
3.3 Electron Configurations and the Periodic Table

For atoms with two or more electrons:

- electrons in different orbitals with the same *n* value have different energies.
- electrons within a sublevel have the same energy.

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < \ldots$



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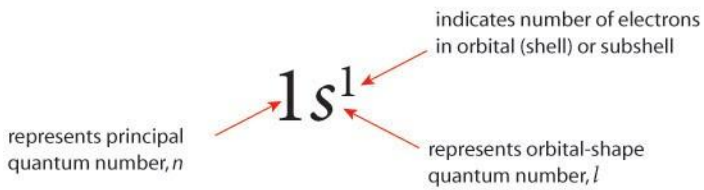
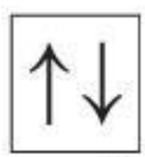
Representing Electrons: Electron Configurations and Orbital Diagrams

The **electron configuration** for an atom shows the number and arrangement of its electrons, in the ground state.



The electron configuration for hydrogen

An **orbital diagram** uses boxes or lines to represent orbitals at each *n* and shows electron spin.



$1s^2$

Orbital diagrams often accompany electron configurations.

? Identify the atom.

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Describing the Electrons in Lithium

The lithium atom has three electrons:

- The first two electrons occupy the 1*s* orbital (n = 1)
- The third electron is at an n = 2 energy level
- l can be 0 or 1; l = 0 (*s*) is lower in energy than l = 1 (*p*)

Atom	Electron	Quantum Numbers	Electron Configuration	Orbital Diagram
lithium	First	$n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$	$1s^2 2s^1$	[↑↓] [↑] [ ][ ][ ] 1*s* 2*s* 2*p*
	Second	$n = 1, l = 0, m_l = 0, m_s = -\frac{1}{2}$		
	Third	$n = 2, l = 0, m_l = 0, m_s = +\frac{1}{2}$		

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Writing Electron Configurations and Orbital Diagrams

Follow the **aufbau principle:**
"build up" electronic configurations of atoms in order of increasing atomic number

Guidelines for "Filling" Orbitals

1. Place electrons into the orbitals in order of increasing energy level.
2. Completely fill orbitals of the same energy level before proceeding to the next orbital or series of orbitals.
3. When electrons are added to orbitals of the same energy sublevel, each orbital receives one electron before any pairing occurs.
4. When electrons are added individually to different orbitals of the same energy, the electrons must all have the same spin.

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Filling Orbitals for Periods 1 and 2

- Boxes in orbital diagrams are written and filled from left to right (increasing energy of orbitals)
- For C apply Hund's rule and for O apply Pauli exclusion principle

Atomic Number (Z)	Element	Orbital Diagram	Electron Configuration
1	H	$\underset{1s}{\boxed{\uparrow}}$	$1s^1$
2	He	$\underset{1s}{\boxed{\uparrow\downarrow}}$	$1s^2$
3	Li	$\underset{1s}{\boxed{\uparrow\downarrow}}\ \underset{2s}{\boxed{\uparrow}}\ \underset{2p}{\boxed{}\boxed{}\boxed{}}$	$1s^2\,2s^1$
4	Be	$\underset{1s}{\boxed{\uparrow\downarrow}}\ \underset{2s}{\boxed{\uparrow\downarrow}}\ \underset{2p}{\boxed{}\boxed{}\boxed{}}$	$1s^2\,2s^2$
5	B	$\underset{1s}{\boxed{\uparrow\downarrow}}\ \underset{2s}{\boxed{\uparrow\downarrow}}\ \underset{2p}{\boxed{\uparrow}\boxed{}\boxed{}}$	$1s^2\,2s^2\,2p^1$
6	C	$\underset{1s}{\boxed{\uparrow\downarrow}}\ \underset{2s}{\boxed{\uparrow\downarrow}}\ \underset{2p}{\boxed{\uparrow}\boxed{\uparrow}\boxed{}}$	$1s^2\,2s^2\,2p^2$

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LEARNING CHECK

Write the electron configurations and draw orbital diagrams for N and F.

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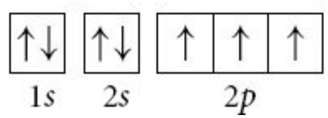
?

Answer on the next slide

LEARNING CHECK

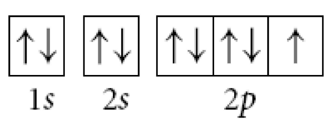
For nitrogen:

$1s^2 2s^2 2p^3$



For fluorine:

$1s^2 2s^2 2p^5$



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Filling Orbitals for Period 3

- Follow the same guidelines as done for Period 1 and 2 elements
- Use condensed electron configuration and corresponding partial orbital diagrams

Full for Z = 11:
$1s^2 2s^2 2p^6 3s^1$

Condensed for Z = 11:
$[Ne]3s^1$

For filling orbitals for transition and Group 12 elements:

- Keep in mind that the order of orbital energies is

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < \ldots$$

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Filling Orbitals for Period 4

Follow the same guidelines up to $Z = 23$. After that, two exceptions are Cr $[Ar]4s^1 3d^5$ and Cu $[Ar]4s^1 3d^{10}$

Atomic Number (Z)	Element	Orbital Diagram	Condensed Electron Configuration
19	K	4s: [↑] 3d: [ ][ ][ ][ ][ ] 4p: [ ][ ][ ]	$[Ar]4s^1$
20	Ca	[↑↓] [ ][ ][ ][ ][ ] [ ][ ][ ]	$[Ar]4s^2$
21	Sc	[↑↓] [↑][ ][ ][ ][ ] [ ][ ][ ]	$[Ar]4s^2 3d^1$
22	Ti	[↑↓] [↑][↑][ ][ ][ ] [ ][ ][ ]	$[Ar]4s^2 3d^2$
23	V	[↑↓] [↑][↑][↑][ ][ ] [ ][ ][ ]	$[Ar]4s^2 3d^3$
24	Cr	[↑] [↑][↑][↑][↑][↑] [ ][ ][ ]	$[Ar]4s^1 3d^5$
25	Mn	[↑↓] [↑][↑][↑][↑][↑] [ ][ ][ ]	$[Ar]4s^2 3d^5$
26	Fe	[↑↓] [↑↓][↑][↑][↑][↑] [ ][ ][ ]	$[Ar]4s^2 3d^6$

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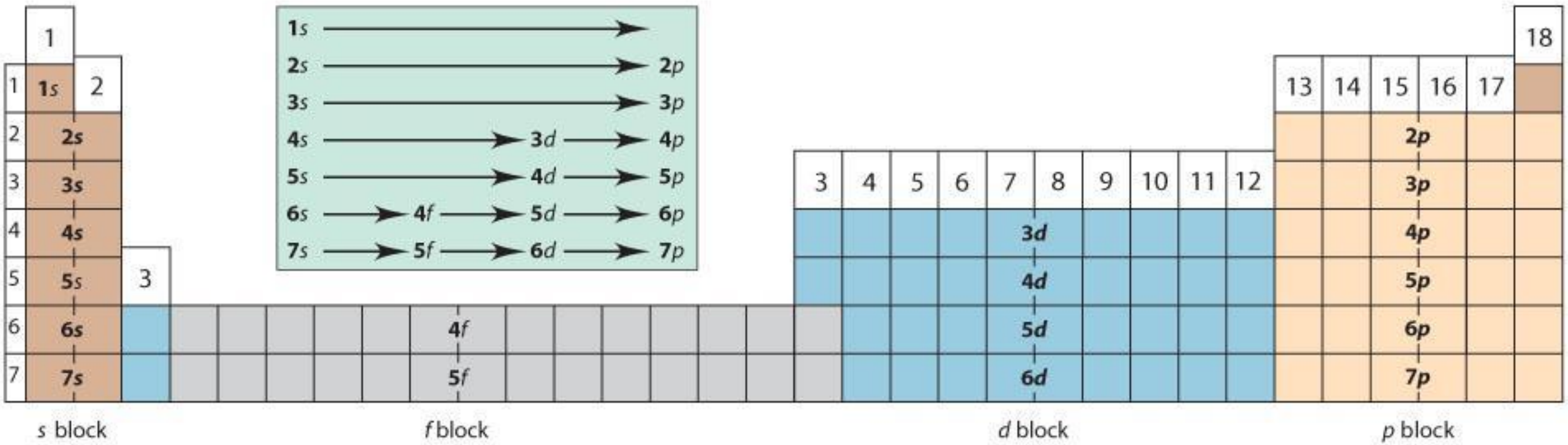
Using the Periodic Table to Predict Electron Configurations



Based on the filling pattern of orbitals, the periodic table can be divided into *s* block, *p* block, *d* block, and *f* block regions.

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Group and Period Numbers Provide Patterns

Elements in a group have similar electron configurations and the same number of valence electrons. Patterns include:

- The last numeral of the group number is the same as the number of valence electrons for main group elements (He is an exception).
- The value of *n* for the highest occupied orbital is the period number.
- At a given energy level, the total number of orbitals is n^2 and the maximum number of electrons is $2n^2$.

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LEARNING CHECK

The condensed electron configuration for silicon is [Ne]$3s^2 3p^2$.

Without using a periodic table, identify the group number, period number, and orbital block for silicon.

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Answer on the next slide

LEARNING CHECK

Group 14, Period 3, *p* block

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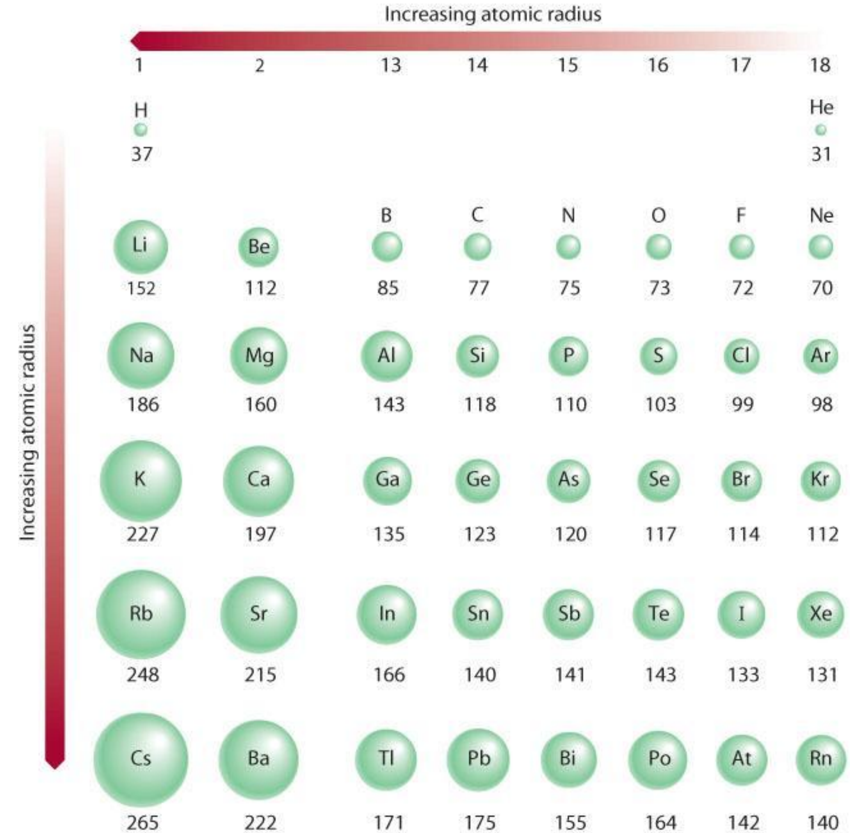
Electron Configurations and Periodic Trends in Atomic Properties

Patterns of electron configurations in the periodic table are related to periodic trends.

Atomic radius trend:

- For main group elements, generally a decrease across a period and an increase down a group.



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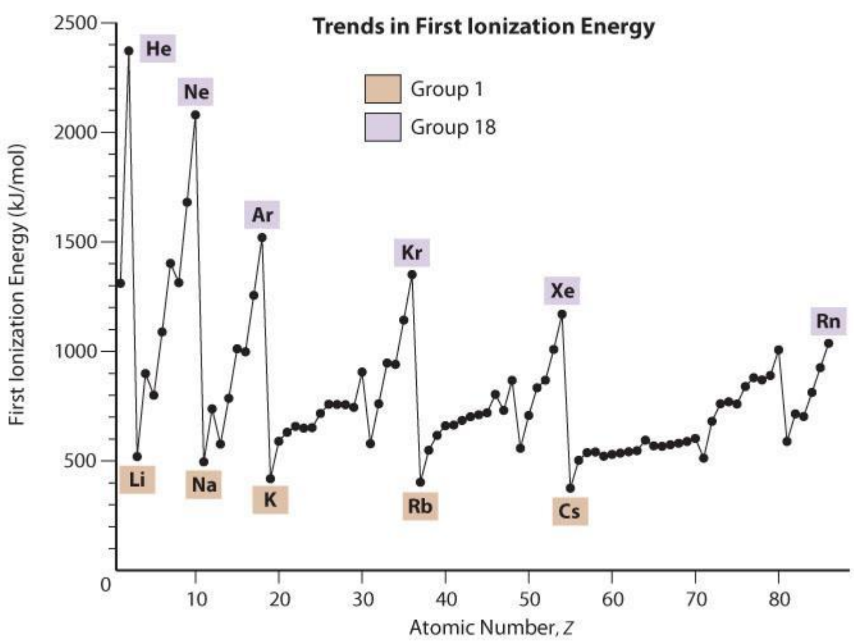
Electron Configurations and Periodic Trends in Atomic Properties

First **ionization energy** is the energy required to remove the first electron from an atom.

- Within a group, it generally decreases as you move down the group.
- Within a period, it generally increases as you move from left to right.



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Electron Configurations and Periodic Trends in Atomic Properties

Electron affinity:

- Trend is more irregular
- In combination with ionization energy, there are trends
  - atoms high in both electron affinity and ionization energy easily form anions
  - atoms low in both easily form cations
  - atoms with very high ionization energies and very low electron affinities do not bond (noble gases)

Electron Affinities

1	2	3	4	5	6	7	8
H – 72.8							He (0.0)
Li – 59.6	Be ≤0	B – 26.7	C – 122	N +7	O – 141	F – 328	Ne (+29)
Na – 52.9	Mg ≤0	Al – 42.5	Si – 134	P – 72.0	S – 200	Cl – 349	Ar (+35)
K – 48.4	Ca –2.37	Ga – 28.9	Ge – 119	As – 78.2	Se – 195	Br – 325	Kr (+39)
Rb – 46.9	Sr –5.03	In – 28.9	Sn – 107	Sb – 103	Te – 190	I – 295	Xe (+41)
Cs – 45.5	Ba –13.95	Tl – 19.3	Pb – 35.1	Bi – 91.3	Po – 183	At – 270	Rn (+41)

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Section 3.3 Review

Section 3.3 Electron Configurations and the Periodic Table

The quantum mechanical model of the atom explains the experimentally determined, electronic structure of the periodic table and the properties of its elements.

Key Terms

atomic radius	ionization energy
aufbau principle	Hund's rule
electron affinity	orbital diagram
electron configuration	

Key Concepts

- For hydrogen, the relative energies of the atomic orbitals depend only on the principal quantum number, *n*. For many-electron atoms, other factors such as the orbital-shape quantum number, *l*, influence the relative energies of atomic orbitals.
- Electron configuration notation and orbital diagrams are two methods commonly used to represent or describe the distribution of electrons in atoms.
- Applying the Pauli exclusion principle, Hund's rule, and the aufbau principle, the electron configuration of atoms can be built up according to the position of the element in the periodic table.
- The modern, quantum mechanical model of the atom enables us to understand the elements, their positions in the periodic table, and their chemical and physical properties based on their electron configuration.

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