

Chapter 11

Modern Atomic Theory



Rutherford's Atom

Nuclear Model of the Atom

- The atom has a small dense nucleus which
 - is positively charged.
 - contains protons (+1 charge).
 - contains neutrons (no charge).
- The remainder of the atom
 - is mostly empty space.
 - contains electrons (-1 charge).



• The nuclear charge (*n*+) is balanced by the presence of *n* electrons moving in some way around the nucleus.



- What are the electrons doing?
- How are the electrons arranged and how do they move?

Electromagnetic Radiation

• One of the ways that energy travels through space.



Electromagnetic Radiation

Characteristics

 Wavelength (λ) – distance between two peaks or troughs in a wave.



Electromagnetic Radiation

Characteristics

- Frequency (v) number of waves (cycles) per second that pass a given point in space
- Speed (c) speed of light (2.9979 × 10⁸ m/s)

$$c = \lambda v$$

Electromagnetic Radiation

Dual Nature of Light

- Wave
- Photon packet of energy





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Electromagnetic Radiation

Different Wavelengths Carry Different Amounts of Energy



Emission of Energy by Atoms

- Atoms can give off light.
 - They first must receive energy and become excited.
 - The energy is released in the form of a photon.
 - The energy of the photon corresponds exactly to the energy change experienced by the emitting atom.



The Energy Levels of Hydrogen

- Atomic states
 - Excited state atom with excess energy
 - Ground state atom in the lowest possible state
- When an H atom absorbs energy from an outside source it enters an excited state.



corresponds exactly to the energy lost by each excited atom.

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excited (to possess excess energy).

The Energy Levels of Hydrogen

Energy Level Diagram

• Energy in the photon corresponds to the energy used by the atom to get to the excited state.





The Energy Levels of Hydrogen

 Only certain types of photons are produced when H atoms release energy. Why?



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The Energy Levels of Hydrogen

Quantized Energy Levels

• Since only certain energy changes occur, the H atom must contain discrete energy levels.



The Energy Levels of Hydrogen

Quantized Energy Levels

• The energy levels of *all* atoms are quantized.





A ramp varies continously in elevation.

A flight of stairs allows only certain elevations; the elevations are quantized.



The Energy Levels of Hydrogen



Concept Check

Why is it significant that the color emitted from the hydrogen emission spectrum is not white?

How does the emission spectrum support the idea of quantized energy levels?



The Energy Levels of Hydrogen



Concept Check

When an electron is excited in an atom or ion

- a) only specific quantities of energy are released in order for the electron to return to its ground state.
- b) white light is never observed when the electron returns to its ground state.
- c) the electron is only excited to certain energy levels.
- d) All of the above statements are true when an electron is excited.

The Bohr Model of the Atom

- Quantized energy levels
- Electron moves in a circular orbit.
- Electron jumps between levels by absorbing or emitting a photon of a particular wavelength.



The Bohr Model of the Atom

- Bohr's model of the atom was incorrect.
 - Electron does not move in a circular orbit.

The Wave Mechanical Model of the Atom

Orbitals

- Nothing like orbits
- Probability of finding the electron within a certain space
- This model gives no information about when the electron occupies a certain point in space or how it moves.



The Hydrogen Orbitals

Orbitals

- Orbitals do not have sharp boundaries.
- Chemists arbitrarily define an orbital's size as the sphere that contains 90% of the total electron probability.



The Hydrogen Orbitals

Hydrogen Energy Levels

- Hydrogen has discrete energy levels.
 - Called principal energy levels
 - Labeled with whole numbers



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The Hydrogen Orbitals

Hydrogen Energy Levels

- Each principal energy level is divided into sublevels.
 - Labeled with numbers and letters
 - Indicate the shape of the orbital



The Hydrogen Orbitals

Hydrogen Energy Levels

• The s and p types of sublevel



The Hydrogen Orbitals

Orbital Labels

- 1. The number tells the principal energy level.
- 2. The letter tells the shape.
 - The letter *s* means a spherical orbital.
 - The letter p means a two–lobed orbital. The x, y, or z subscript on a p orbital label tells along which of the coordinate axes the two lobes lie.

The Hydrogen Orbitals

Hydrogen Orbitals

- Why does an H atom have so many orbitals and only 1 electron?
 - An orbital is a potential space for an electron.
 - Atoms can have many potential orbitals.

The Wave Mechanical Model: Further Development

Atoms Beyond Hydrogen

- The Bohr model was discarded because it does not apply to all atoms.
- Atoms beyond hydrogen have an equal number of protons and electrons.
 - Need one more property to determine how the electrons are arranged
 - Spin electron spins like a top

Atoms Beyond Hydrogen

 Pauli Exclusion Principle – an atomic orbital can hold a maximum of 2 electrons and those 2 electrons must have opposite spins.

Principal Components of the Wave Mechanical Model of the Atom

- Atoms have a series of energy levels called principal energy levels, which are designated by whole numbers (n = 1, 2, 3, etc.).
- 2. The energy of the level increases as the value of *n* increases.
- 3. Each principal energy level contains one or more types of orbitals, called sublevels.
- 4. The number of sublevels present in a given principal energy level equals *n*.

Principal Components of the Wave Mechanical Model of the Atom

- 5. The *n* value is always used to label the orbitals of a given principal level and is followed by a letter that indicates the type (shape) of the orbital (1*s*, 3*p*, etc.).
- An orbital can be empty or it can contain one or two electrons, but never more than two. If two electrons occupy the same orbital, they must have opposite spins.

Principal Components of the Wave Mechanical Model of the Atom

7. The shape of an orbital does not indicate the details of electron movement. It indicates the probability distribution for an electron residing in that orbital.

The Wave Mechanical Model: Further Development



Concept Check

Which of the following statements **best** describes the movement of electrons in a *p* orbital?

- a) The electron movement cannot be exactly determined.
- b) The electrons move within the two lobes of the *p* orbital, but never beyond the outside surface of the orbital.
- c) The electrons are concentrated at the center (node) of the two lobes.
- d) The electrons move along the outer surface of the *p* orbital, similar to a "figure 8" type of movement.

Electron Arrangements in the First Eighteen Atoms on the Periodic Table

H Atom

- Electron configuration electron arrangement
 1s¹
- Orbital diagram orbital is a box grouped by sublevel containing arrow(s) to represent electrons



Electron Arrangements in the First Eighteen Atoms on the Periodic Table

Li Atom

- Electron configuration $1s^2 2s^1$
- Orbital diagram

 $1s^22s^1$





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Electron Arrangements in the First Eighteen Atoms on the Periodic Table

O Atom

• The lowest energy configuration for an atom is the one having the maximum number of unpaired electrons in a particular set of degenerate (same energy) orbitals.



Electron Arrangements in the First Eighteen Atoms on the Periodic Table

• The electron configurations in the sublevel last occupied for the first eighteen elements.



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Electron Arrangements in the First Eighteen Atoms on the Periodic Table

Classifying Electrons

- Core electrons inner electrons
- Valence electrons electrons in the outermost (highest) principal energy level of an atom
 - $1s^22s^22p^6$ (valence electrons = 8)
 - The elements in the same group on the periodic table have the same valence electron configuration.
 - Elements with the same valence electron arrangement show very similar chemical behavior.

Electron Arrangements in the First Eighteen Atoms on the Periodic Table



Concept Check

How many unpaired electrons does the element cobalt (Co) have in its lowest energy state?

Electron Arrangements in the First Eighteen Atoms on the Periodic Table



Concept Check

Can an electron in a phosphorus atom ever be in a 3*d* orbital? Choose the best answer.

a) Yes. An electron can be excited into a 3*d* orbital.

- b) Yes. A ground-state electron in phosphorus is located in a 3*d* orbital.
- c) *No*. Only transition metal atoms can have electrons located in the *d* orbitals.
- d) *No*. This would not correspond to phosphorus' electron arrangement in its ground state.

Electron Configurations and the Periodic Table

• Look at electron configurations for K through Kr.



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Electron Configurations and the Periodic Table

Orbital Filling and the Periodic Table



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Electron Configurations and the Periodic Table

Orbital Filling

- 1. In a principal energy level that has *d* orbitals, the *s* orbital from the next level fills before the *d* orbitals in the current level.
- 2. After lanthanum, which has the electron configuration [Xe] $6s^25d^1$, a group of fourteen elements called the lanthanide series, or the lanthanides, occurs. This series of elements corresponds to the filling of the seven 4*f* orbitals.

Electron Configurations and the Periodic Table

Orbital Filling

3. After actinum, which has the configuration $[Rn]7s^26d^1$, a group of fourteen elements called the actinide series, or actinides, occurs. This series corresponds to the filling of the seven 5*f* orbitals.

Electron Configurations and the Periodic Table

Orbital Filling

4. Except for helium, the group numbers indicate the sum of electrons in the *ns* and *np* orbitals in the highest principal energy level that contains electrons (where *n* is the number that indicates a particular principal energy level). These electrons are the valence electrons.

Electron Configurations and the Periodic Table



Exercise

Determine the expected electron configurations for each of the following. a) S 1s²2s²2p⁶3s²3p⁴ or [Ne]3s²3p⁴ b) Ba [Xe]6s² c) Eu [Xe]6s²4f⁷

Atomic Properties and the Periodic Table

Metals and Nonmetals

- Metals tend to lose electrons to form positive ions.
- Nonmetals tend to gain electrons to form negative ions.



Metalloids

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Atomic Properties and the Periodic Table

Ionization Energy

- Energy required to remove an electron from a gaseous atom or ion.
 - $X(g) \rightarrow X^+(g) + e^-$

$$\begin{split} \text{Mg} &\to \text{Mg}^{+} + e^{-} & \text{I}_{1} = 735 \text{ kJ/mol} & (1^{\text{st}} \text{ IE}) \\ \text{Mg}^{+} &\to \text{Mg}^{2+} + e^{-} & \text{I}_{2} = 1445 \text{ kJ/mol} & (2^{\text{nd}} \text{ IE}) \\ \text{Mg}^{2+} &\to \text{Mg}^{3+} + e^{-} & \text{I}_{3} = 7730 \text{ kJ/mol} & *(3^{\text{rd}} \text{ IE}) \end{split}$$

*Core electrons are bound much more tightly than valence electrons.

Atomic Properties and the Periodic Table

Ionization Energy

- In general, as we go across a period from left to right, the first ionization energy increases.
- Why?
 - Electrons added in the same principal quantum level do not completely shield the increasing nuclear charge caused by the added protons.
 - Electrons in the same principal quantum level are generally more strongly bound from left to right on the periodic table.

Atomic Properties and the Periodic Table

Ionization Energy

Energy required to remove an electron increases

Period



Ionization energies generally increase across a period

Atomic Properties and the Periodic Table

Ionization Energy

- In general, as we go down a group from top to bottom, the first ionization energy decreases.
- Why?
 - The electrons being removed are, on average, farther from the nucleus.

Atomic Properties and the Periodic Table

Ionization Energy



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Atomic Properties and the Periodic Table



Concept Check

Which atom would require more energy to remove an electron? Why? Na CI



Atomic Properties and the Periodic Table



Concept Check

Which atom would require more energy to remove an electron? Why?



Atomic Properties and the Periodic Table

Atomic Size

- In general as we go across a period from left to right, the atomic radius decreases.
 - Effective nuclear charge increases, therefore the valence electrons are drawn closer to the nucleus, decreasing the size of the atom.
- In general atomic radius increases in going down a group.
 - Orbital sizes increase in successive principal quantum levels.

Atomic Properties and the Periodic Table

Relative Atomic Sizes for Selected Atoms





Atomic Properties and the Periodic Table



Concept Check

Which should be the larger atom? Why? Na Cl



Atomic Properties and the Periodic Table



Concept Check

Which should be the larger atom? Why? Li Cs

Atomic Properties and the Periodic Table



Concept Check

Which is larger?

- The hydrogen 1s orbital
- The lithium 1s orbital

Which is lower in energy?

- •The hydrogen 1s orbital
- •The lithium 1s orbital

Atomic Properties and the Periodic Table



Exercise

Arrange the elements oxygen, fluorine, and sulfur according to increasing:

Ionization energy

S, O, F

Atomic size

F, O, S