Ch 7: Atomic Electron Configurations & Chemical Periodicity

1. Electron Spin & Pauli Exclusion Principle
2. Polyelectronic Atoms
3. Electron Configurations
4. Ionic Electron Configurations
5. Periodic Trends & Chemical Properties
7.1 Pauli Exclusion Principle

Two Electrons Can Occupy an Orbital According to the **Pauli Exclusion Principle**

**Note: Electrons Have Intrinsic Spin**

-A Spinning Charged Particle Creates a Magnetic Field, and Just Like Two Magnets, Will Repel Unless North-South Pole Coupled, **Two Electrons Must Have Opposite Spins to Be in the Same Orbit**

\[ m_s \text{ – fourth quantum number} \]
Summary of Quantum numbers

-Electrons can be described by orbitals which can in turn be described by 4 quantum numbers

-No two electrons can have the same set of quantum numbers

$n$ – Principle Q# - describes “shell”

$l$ – angular momentum Q# - describes shape

$m_l$ – magnetic Q# - describes orientation

$m_s$ – spin Q# - describes intrinsic spin
Periodic Table & Quantum Numbers
7.2 Polyelectronic Atoms

Previous treatment was for “Hydrogen Like Atom” in that we do not consider electron/electron interactions.

Core Electrons **Shield** Valence Electrons From Nucleus, Reducing the Effective Nuclear Charge

Lifts degeneracy as function of principle quantum number
Orbital Energies for Multiple Electron Atoms

The 4s orbital “penetrates” the 3d orbital and feels a greater effective nuclear charge ($Z^*$)
Comparing Energy Levels of H-like to Polyatomic Atom

Orbital Energies for Hydrogen

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<th>3s</th>
<th>3p</th>
<th>3d</th>
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<td>n=2</td>
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<tr>
<td>n=1</td>
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Orbital Energies for Multiple Electron Atoms

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<td>1s</td>
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note the energy of an orbital only depends on n

All orbitals of same n are said to be degenerate, that is to have the same energy

the 4s orbital “penetrates” the 3d orbital and feels a greater effective nuclear charge
7.3 Electron Configurations

General Rules

1. Electrons Fill Lowest Energy Orbitals First (Aufbau Principle)

So First We Need to Determine the Order Of Orbital Energies
Electron Configurations

General Rules

1. Electrons Fill Lowest Energy Orbitals First (Aufbau Principle)
Electron Configurations

General Rules

1. Electrons Fill Lowest Energy Orbitals First (Aufbau Principle)

2. For Degenerate Orbitals (Equal Energy), Fill Each Orbital With One $e^-$ Before Placing 2 $e^-$ in an Orbital (Hunds Rule)

\[
\begin{array}{ccc}
\uparrow & \uparrow & \_ \\
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\end{array}
\quad
\begin{array}{ccc}
\uparrow \downarrow & \_ & \_ & \_ \\
\_ & \_ & \_ \\
\end{array}
\]

(wrong)
Electron Configurations

General Rules

1. Electrons Fill Lowest Energy Orbitals First (Aufbau Principle)

2. For Orbitals of Equal Energy, Fill Each Orbital With One e\textsuperscript{-} Before Placing 2 in an Orbital (Hunds Rule)

3. Each Orbital Can Only Have Two Electrons of Opposite Spin (Pauli Exclusion Principle)

4. Determine # of Electrons in Atom (or Ion), and Fill the Orbitals According to the Above Rules
Electron Configuration of Hydrogen

Number of electrons = 1

H: 1s^1

Principle Quantum #: 1

Azimuthal Quantum #: 1

1s Quantum #: 1

Energy: 4p, 3p, 2p, 3s, 4s
Electron Configuration of Helium

Number of electrons = 2

He: 1s²

Energy:

1s

2s

3s

3p

4s

4p

3d
Electron Configuration of Lithium

Number of electrons = 3

Li: 1s\(^2\)2s\(^1\)

Inner Shell

Valence Shell

Energy->

1s
2s
2p\(_x\)
2p\(_y\)
2p\(_z\)

4p
3d
4s
3p
3s
2p
1s
Electron Configuration of Beryllium

Number of electrons = 4

Be: \(1s^22s^2\)
Electron Configuration of Boron

Number of electrons = 5

B: ${1s}^2{2s}^2{2p}^1$
Electron Configuration of Carbon

Number of electrons = 6

C: $1s^22s^22p^2$

Hund's Rule
Electron Configuration of Nitrogen

Number of electrons = 7

N: 1s^2 2s^2 2p^3
Electron Configuration of Oxygen

Number of electrons = 8

O: $1s^2 2s^2 2p^4$
Electron Configuration of Fluorine

Number of electrons = 9

F: 1s\(^2\)2s\(^2\)2p\(^5\)
Electron Configuration of Neon

Number of electrons = 10

Ne: 1s²2s²2p⁶

Energy:

1s  2s  2pₓ  2pᵧ  2pₜ  3s  3p  4s  4p  3d

↓↓  ↓↓  ↓↓  ↓↓  ↓↓  ↓↓  ↓↓  ↓↓  ↓↓  ↓↓
Electron Configuration of Sodium (11 electrons)

Na: $1s^22s^22p^63s^1$

Inner Shell (Core) Orbitals

Valence Shell (Orbital)

Inner Shells can be abbreviated by Nobel gas they represent (Ne= $1s^22s^22p^6$)

Alternative (preferred) Notation use Nobel gas symbol to represent Core Electrons

Na: [Ne]$3s^1$
Note the Core Electrons Are Not Involved in Bonding, What Does This Tell Us About the Alkali Metals?

Write Electron Configurations of The Halogens, Can You Draw Any Predictions in Behavior Based on These Configurations?
Write the Electron Configuration of Vanadium and Chromium

V: \([\text{Ar}]4s^23d^3\)

Cr: \([\text{Ar}]4s^13d^5\)

Why isn’t Chromium \([\text{Ar}]4s^23d^4\)?
Order of Orbital Energies

Filled and 1/2 Filled Sublevels Are Exceptionally Stable, This Is the Reason Behind the Stability of Noble Gasses and the Previous Electron Configuration of Chromium.

Cr: [Ar]$4s^13d^5$
7.4 Electron Configuration of Ions

1. Anions – Add electrons to Lowest Energy Unoccupied Orbital

   - Tend to form ions which are isoelectronic to nearest noble gas

   \[ \text{S}^-^2 : [\text{Ne}]3s^23p^6 \]
   \[ \text{P}^-^3 : [\text{Ne}]3s^23p^6 \]
Electron Configuration of Ions

1. Cations – Remove electrons the orbital which is furthest from the nucleus (note how the 4s is both closer and further from the nucleus than the 3d

V: [Ar]4s²3d³

What is V⁺²?

V⁺²: [Ar]3d³
Ionic Radii

Anions Are Larger Than Parent Atom
Ionic Radii

Cations Are Smaller Than Parent Atom
7.5 Periodic Trends in Atomic Properties

1. Ionization Energy - ease of loosing an electron
2. Electron Affinity – ease of gaining an electron
3. Atomic radii – “size of atom”
Atomic Radii

How are atomic radii determined?

1/2 the Internuclear Bond Length for a Homonuclear Bond

\[ \text{Atomic Radii of Carbon} = 0.77 \ \text{Å} \]
Atomic Size
Atomic Size

What 2 Factors Influence Atomic Size?

1. **n - Principle quantum #:** as n increases, the orbitals increase in size

Hydrogen

1s

r

ψ²

n=1 (first shell)
Atomic Size

What 2 Factors Influence Atomic Size?

1. **n - Principle quantum #:** as n increases, the orbitals increase in size

Lithium

Notice how the 1s radii shrinks as the nuclear charge increases
Atomic Size

What 2 Factors Influence Atomic Size?

1. **n - Principle quantum #:** as \( n \) increases, the orbitals increase in size

Sodium

- **Core Electrons (inner shell):** 1s, 2s, 3s
- **Valence Electrons (outer shell):** 3s

\( n = 3 \) (third shell)
Atomic Size

What 2 Factors Influence Atomic Size?

1. **n - Principle quantum #:** as n increases, the orbitals increase in size

2. **Effective Nuclear Charge:** Core electrons shield valence electrons from the nucleus thus reducing the positive charge the valence electron feels
Atomic Size

Why Do Atoms Get Larger Going Down a Group?

\( n \) increases

Why do Atoms Get Smaller Going Across a Period?

The effective nuclear charge goes up as the \# of protons increase, while the \# of core electrons stays constant, so the valence electrons are pulled in tighter.
First Ionization Energy

- the amount of energy required to remove an electron from a gas phase atom (forming a cation)

\[ M(g) \rightarrow M^+(g) + e^- \]
First Ionization Energy

Why does the ionization energy tend to increase going across a period?

The effective nuclear charge increases, making it harder to remove an electron
First Ionization Energy

Why does the ionization energy decrease going Be to B and Mg to Al?

The 2s or 3s orbitals are respectively filled and have a partial shielding effect on the 2p\(^1\) & 3p\(^1\) electrons of B & Al.

(Decreasing the effective nuclear charge)
First Ionization Energy

Why Does the Ionization Energy Tend to Decrease in Going From N to O & P to S?

The spin pairing energy associated with 2 electrons in a single orbital of the ns\(^2\)np\(^4\) electron configuration is repulsive and weakens the nuclear attraction
First Ionization Energy

Why Does the Ionization Energy Decrease Going Down a Group?

The Valence Electron Tends to Be Further From the Nucleus, Making It Easier to Be Removed
Higher Ionization Energies

Note: You can move more than one electron from an atom

First Ionization Energy

\[ \text{M(g)} \rightarrow \text{M}^+ \text{(g)} + e^- \]

Second Ionization Energy

\[ \text{M}^+ \text{(g)} \rightarrow \text{M}^{+2} \text{(g)} + e^- \]

Which is Larger?
**Higher Ionization Energies**

First Ionization Energy

$$\text{Li}(g) \rightarrow \text{Li}^+(g) + e^- \quad I_1 = 513.3 \text{ kJ/mol}$$

Second Ionization Energy

$$\text{Li}^+(g) \rightarrow \text{Li}^{2+}(g) + e^- \quad I_2 = 7298 \text{ kJ/mol}$$
### Higher Ionization Energies

**TABLE 6.1**  
Successive Ionization Energies (kJ/mol) for Third-Row Elements

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<thead>
<tr>
<th>$E_i$ Number</th>
<th>Na</th>
<th>Mg</th>
<th>Al</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cl</th>
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<td>$E_{i1}$</td>
<td>496</td>
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Ionization Energy

Concept Question

Is It Easier to Ionize an Element With a High or a Low Ionization Energy?
Electron Affinity, $E_{ea}$

The Energy Change Associated With the Formation of an Anion From a Neutral Gas Phase Atom

$$\text{A}(g) + e^-(g) \rightarrow \text{A}^-(g)$$

Note, Electron Affinities Can Be Both Endothermic and Exothermic.

What Does an Positive Electron Affinity Mean?
Electron Affinities

Energy must be added for the reaction to proceed.

Ar ([Ne]:3s^23p^6) + e^- + ENERGY $\rightarrow$ Ar^-([Ne]:3s^23p^64s^1)

What Does a Negative Electron Affinity Mean?

Energy is Released

Cl ([Ne]:3s^23p^5) + e^- $\rightarrow$ Cl^-([Ne]:3s^23p^6) + ENERGY
Periodic Trends: Electron Affinity

Electron Affinity Tends to Decrease Going Across a Period With Some Notable Exceptions (becoming more exothermic)
Periodic Trends: Electron Affinity

**Why is group IIA > IA?**

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Group IIA has a filled s orbital
Periodic Trends: Electron Affinity

Why is group VA > IVA?

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Group VA has a 1/2 filled p shell
Periodic Trends: Electron Affinity

**Why is group VIIIA Positive?**

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The e⁻ is being added to the next shell which is shielded from the nucleus.
Noble Gases

Which Group Tends to Have the Highest Ionization Energy?

Noble Gases, - Thus They Do Not Want to Lose Electrons (Get Oxidized)

Which Group Tends to Have the Highest Electron Affinity?

Noble Gases, - Thus They Do Not Want to Gain Electrons (Get Reduced)
Metals

Tend to Have Low Ionization Energies

- Easily Oxidized (lose electrons)
- Form Cations

Charge of cations can be determined by successive ionization energies (table 7.2)
Nonmetals

- Tend to have low (negative) electron affinities

  - Easily Reduced (gain electrons)

  - Tend to Form anions

Note: Noble gases are an exception