Atomic Orbitals

Objectives

1. To learn about the shapes of the $s$, $p$ and $d$ orbitals
2. To review the energy levels and orbitals of the wave mechanical model of the atom
3. To learn about electron spin
A. Electron Location

- Energy Level
  - Called principal energy levels
  - Corresponds to row on periodic table
  - As n increases, E increases and the electron is farther away from the nucleus
A. Electron Location

- Sublevel
  - Shape of electron cloud
    - s = spherical
    - p = dumbbell
    - d = too complex
    - f = too complex

- 1st E level has 1 sublevel -- s
- 2nd E level has 2 sublevels -- s and p
- 3rd E level has 3 sublevels -- s, p, and d
- 4th E level has 4 sublevels -- s, p, d and f
S Sublevel

- Orbitals do not have sharp boundaries.
A. Electron Location

- Orbitals
  - Describes the orientation in space within a sublevel
    - \( s = 1 \) orbital
    - \( p = 3 \) orbitals
    - \( d = 5 \) orbitals
    - \( f = 7 \) orbitals

**ONLY 2 electrons in any orbital!!!**
• The $s$ and $p$ types of sublevel
A. Electron Location

- Spin
  - Electrons in the same orbital must have opposite spins. One spins clockwise and the other spins counter-clockwise. (+1/2, or -1/2)

  ONLY 2 electrons in any orbital!!!
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Atomic Orbitals

d - orbitals
What is the maximum number of electrons found in each of the following?

- 2p orbital _______
- 2p sublevel _______
- 4p sublevel _______
- 3d orbital _______
- E level 1 _______
- E level 3 _______
- any f sublevel _______
- 4s orbital _______
- 2d orbital_______
<table>
<thead>
<tr>
<th>Energy Level</th>
<th># of Sublevels</th>
<th>Total # e / E Level</th>
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</table>
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- Principal level 1: One sublevel
- Principal level 2: Two sublevels
- Principal level 3: Three sublevels
- Principal level 4: Four sublevels
Electron Configuration

The way in which electrons are arranged around the nucleus according to energy specifications.
Electron Configuration

Three rules that dictate how electrons are arranged.

1. **Aufbau Principle** - electrons enter orbitals of lowest energy first. See diagonal chart or periodic table.

   Electrons do not fill in orbitals in consecutive numerical order.
2. **Pauli Exclusion Principle** - an atomic orbital can hold a maximum of 2 electrons and those 2 electrons must have opposite spins.
Electron Configuration

Orbital diagram – orbital is a box grouped by sublevel containing arrow(s) to represent electrons

H: \( 1s^1 \)

Configuration | Orbital diagram
--- | ---

Value of \( n \) (principal energy level) | Type (shape) of orbital
--- | ---

Number of electrons in the orbital

\( 1s^1 \)
3. **Hund’s Rule** - When electrons occupy orbitals of equal energy (same sublevel), one electron enters each orbital with parallel spin before pairing oppositely.

Example: a 2p sublevel with 3 electrons

a 3d sublevel with 8 electrons
He atom

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

Two electrons in 1s orbital

He: $1s^2$
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Atomic Orbitals

Li atom

– Electron configuration – $1s^2\ 2s^1$
– Orbital diagram

Li: $1s^2\ 2s^1$

\[ \begin{array}{c}
\text{Li} \\
1s^2 \ 2s^1 \\
\uparrow \downarrow \ \uparrow \\
\text{Be} \\
1s^2 \ 2s^2 \\
\uparrow \downarrow \ \uparrow \downarrow \\
\end{array} \]
A. Electron Arrangements in the First 18 Atoms on the Periodic Table

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<tr>
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<td>He</td>
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<td>Be</td>
<td>2s(^2)</td>
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<td>1s(^2)</td>
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<td>Mg</td>
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<td>B</td>
<td>2p(^1)</td>
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<td>C</td>
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<td></td>
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<td>Ar</td>
<td>3p(^6)</td>
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</table>
A. Electron Arrangements in the First 18 Atoms on the Periodic Table

Classifying Electrons

- **Valence electrons** – electrons in the outermost (highest) principal energy level of an atom
- **Core electrons** – inner electrons
- Elements with the same valence electron arrangement show very similar chemical behavior.
B. Electron Configurations and the Periodic Table

- Look at electron configurations for K through Kr

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| K | 4s$^1$ | Ca | 4s$^2$ | Sc | 3d$^1$ | Ti | 3d$^2$ | V | 3d$^3$ | Cr | 4s$^1$3d$^5$ | Mn | 3d$^5$ | Fe | 3d$^6$ | Co | 3d$^7$ | Ni | 3d$^8$ | Cu | 4s$^1$3d$^{10}$ | Zn | 3d$^{10}$ | Ga | 4p$^1$ | Ge | 4p$^2$ | As | 4p$^3$ | Se | 4p$^4$ | Br | 4p$^5$ | Kr | 4p$^6$ |
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Atomic Orbitals

B. Electron Configurations and the Periodic Table

- Orbital filling and the periodic table
B. Electron Configurations and the Periodic Table

<table>
<thead>
<tr>
<th>Periodic Table and Electron Configurations</th>
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<tbody>
<tr>
<td>1. The group labels for Groups 1, 2, 3, 4, 5, 6, 7, and 8 indicate the <em>total number</em> of valence electrons for the atoms in these groups. For example, all the elements in Group 5 have the configuration $ns^2np^3$. (Any $d$ electrons present are always in the next lower principal energy level than the valence electrons and so are not counted as valence electrons.)</td>
</tr>
<tr>
<td>2. The elements in Groups 1, 2, 3, 4, 5, 6, 7, and 8 are often called the <strong>main-group elements</strong>, or <strong>representative elements</strong>. Remember that every member of a given group (except for helium) has the same valence-electron configuration, except that the electrons are in different principal energy levels.</td>
</tr>
</tbody>
</table>
C. 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.
C. Atomic Properties and the Periodic Table

Atomic Size

- Size tends to increase down a column. Why?
- Size tends to decrease across a row. Why?
C. Atomic Properties and the Periodic Table

Atomic size

Which is smaller?
C. Atomic Properties and the Periodic Table

**Ion size**

Cations – are smaller than their corresponding neutral atom

Ca or Ca\(^{+2}\)

Li\(^{+1}\) or Li

Anions – are larger than their corresponding neutral atom

Br\(^{-1}\) or Br

S or S\(^{-2}\)
C. Atomic Properties and the Periodic Table

**Ionization Energies**

- **Ionization Energy** – energy required to remove an electron from an individual atom (gas)

  - Tends to decrease down a column
  - Tends to increase across a row
Electronegativity – tendency for an atom to attract electrons to itself when bonded to another element

- Tends to decrease down a column
- Tends to increase across a row
C. Atomic Properties and the Periodic Table

Lewis Dot Structure – shows the valence electrons for an element