3.6 Atomic Structure and the Periodic Table

Bohr's Theory Was Incorrect Because...

- Only explained the line spectrum of hydrogen
- Position and motion of an e^- cannot be specified (since the e^- is so small, cannot locate them exactly)
- An e^- does not move in an "orbit" or circular pattern of fixed radius
- Electrons have properties of both particles (mass) and waves (they can be reflected)

Quantum Mechanics

- Wave mechanics: A type of mathematics used to describe the probability of an electron being in a certain "region of space" around the nucleus at a certain time. (Schrodinger, 1924).
- Orbital: A region of space where an e^- is most likely to be found at a certain time.
- Wave function: The equation that describes the shape of an orbital where e^- are found. (i.e. spherical (s), "dumbbell" (p), etc.)

Creating Energy-Level Diagrams

Aufbau (building up) Principle

- Electrons are added to the lowest energy orbital available.

Pauli Exclusion Principle

- An orbital can be empty, have one electron or have two electrons (at most).

Hund's Rule

- Electrons in the same sub-level will not pair up (occupy the same orbital) until all orbitals in the sub-level are half-filled (have I electron).

Heisenberg Uncertainty Principle

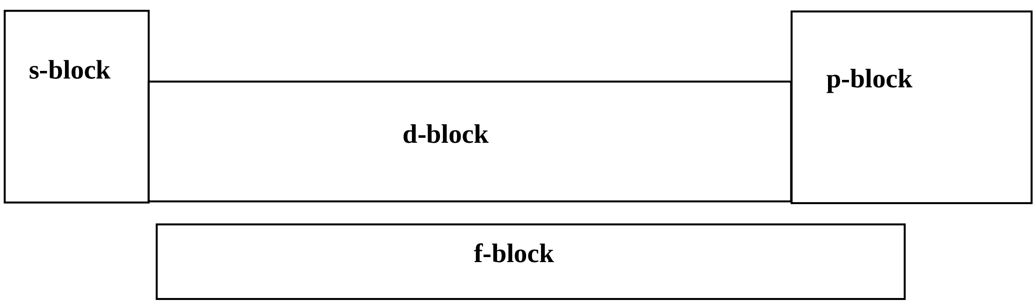
- It is impossible to determine simultaneously the exact momentum and position of an electron. (Therefore, we cannot determine the trajectory of any electron...no orbits!)

Memory Aid for Determining Ground State e^- Configuration

- Complete the table below using figure 5 on page 188.

7s	7p	7d	7f
6s	6p	6d	6f
5s	5p	5d	5f
4s	4p	4d	4f
3s	3p	3d	
2s	2p		
1s			

Periodic Table as Blocks



Remember for Electron Distribution

The maximum number of electrons in a given energy level is $2n^2$.

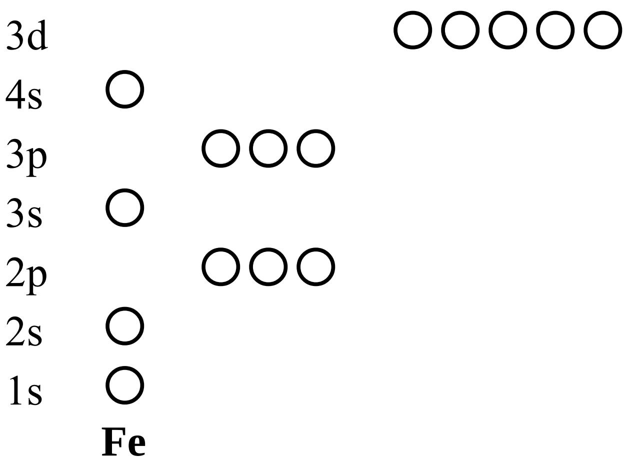
Principle energy level (Principle Quantum Number = *n*)	Number of energy sublevels (Secondary Quantum Number = ℓ)	Type of energy sublevel	Maximum number of electrons for the energy level ($2n^2$)
1	1 (0)	s	2
2	2 (0,1)	s, p	8
3	3 (0,1,2)	s, p, d	18
4	4 (0,1,2,3)	s, p, d, f	32

Only 2 e^- per type of orbital

s orbitals have 2 e^-	therefore 2 e^- in a s orbital
p orbitals have 6 e^-	therefore 2 e^- in a p_x orbital 2 e^- in a p_y orbital 2 e^- in a p_z orbital
d orbitals have 10 e^-	therefore 2 e^- in a d_{xy} orbital 2 e^- in a d_{xz} orbital 2 e^- in a d_{yz} orbital 2 e^- in a $d_{x^2-y^2}$ orbital 2 e^- in a d_{x^2} orbital
f orbitals have 14 e^-	not needed for our purposes

Example of Electron Energy Diagram for Iron (Fe)

- Complete the diagram using Figure 4 on page 188.



Energy Level Diagrams for Anions

- Add the extra electrons corresponding to the ion charge for the anion. (See sample on p. 190)

Energy Level Diagrams for Cations

- Remove electrons from the orbital with the highest principle quantum number. (See sample on p. 190)

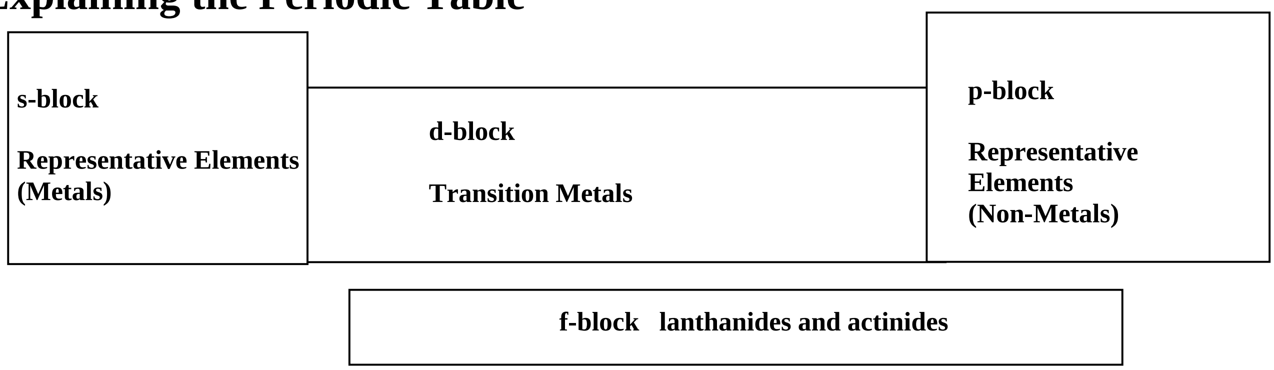
Electron Configurations

Orbital

Principle Quantum Number → $3p^5$ ← Number of electrons in orbital(s)

- A brief method to show the distribution of electrons among the various orbitals in an atom according to quantum mechanics.
- E.g.: Silicon $1s^2 2s^2 2p^6 3s^2 3p^2$ this can be shorted to the nearest noble gas $[Ne]3s^2 3p^2$ (only the electrons in the valence are listed).

Explaining the Periodic Table



Ionic Charges

- Same rules as before
- Cations: Remove electrons from highest energy level
  Zn: $[Ar]\ 4s^2\ 3d^{10}$ $\quad$ Zn^{2+}: $[Ar]\ 3d^{10}$
- Anions: Add electrons to the next energy level
  Cl: $[Ne]\ 3s^2\ 3p^5$ $\quad$ Cl^{1-}: $[Ne]\ 3s^2\ 3p^6$
- More than one possible ion? E.g. Pb +2 and +4
  Pb:$[Xe]\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^2$ $\quad$ Pb^{2+}:$[Xe]\ 6s^2\ 4f^{14}\ 5d^{10}$ $\quad$ Pb^{4+}:$[Xe]\ 4f^{14}\ 5d^{10}$

Magnetism

- Based on electron spin.
- Ferromagnetism: iron, cobalt, nickel → Based on the fact there are unpaired electrons in the valence all with the same spin that contribute to magnetism. Groups of atoms create domains that can be lined up into a permanent magnet.

- Paramagnetism: almost all other elements with an unpaired electron in the valence. They do not create domains and the magnetism is for an individual atom instead of a group of atoms.

Anomalous Electron Configurations

		Predicted Electron Configuration	Actual Electron Configuration
24	Cr	$1s^22s^22p^63s^23p^64s^23d^4$	$1s^22s^22p^63s^23p^64s^13d^5$
29	Cu	$1s^22s^22p^63s^23p^64s^23d^9$	$1s^22s^22p^63s^23p^64s^13d^{10}$

- For an atom to be stable it must be in the lowest possible energy state (ground state). Apparently, the lowest possible energy state for Cr and Cu include 2 partially filled orbitals (breaking of Aufbau's Principle).

Homework
- Practice 1,2,3,4,6,7,8,9,10,11
- Questions 1,2,3,4,5,6,7,8,9,10,11,12,13,14